SHARP INTERFACE MODELS FOR
SOLID STATE DEWETTING
AND THEIR APPLICATIONS

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SHARP INTERFACE MODELS FOR 
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AND THEIR APPLICATIONS 

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DECLARATION

I hereby declare that the thesis is my original work and it has been written by me in its entirety. I have duly acknowledged all the sources of information which have been used in the thesis.

This thesis has also not been submitted for any degree in any university previously.

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Summary

Solid-state dewetting is a ubiquitous physical phenomenon occurring in the solid-solid-vapor system, describing the agglomeration of solid thin films on the substrate. The thin films supported by the substrate are typically unstable and could exhibit complex morphological evolutions, including hole formulation, edge retraction, rim pinch-off and so on, while still remaining the state of solid. The capillary instability is the driving force of this process and makes the thin film moving towards its equilibrium by decreasing the total surface energy. Surface diffusion flow and contact line migration have been recognised as the two main kinetic features for solid-state dewetting.

The aim of this thesis is to develop mathematical models, propose efficient and accurate numerical methods for simulating the solid-state dewetting both in two dimensions and three dimensions. Moreover, extensive numerical simulation results are presented to validate the convergence of the numerical schemes, show consistent morphological evolutions observed in physics experiments, and demonstrate the accuracy of the models.

Firstly, we study the two-dimensional problem via the sharp interface approach, in which the film/vapor interface is assumed to be an open curve with two contact points attached to the substrate. By performing the first and second variation of the
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Secondly, based on the thermodynamic variation, the rigorous derivation of the three-dimensional sharp interface model is presented with the introduction of the speed method and shape derivatives. The equations for the three-dimensional equilibrium shape as well as the anisotropic Young equation are discussed subsequently according to the variation. Similar to the two-dimensional case, the derived sharp interface model includes the surface diffusion flow and relaxed contact angle conditions for describing the surface evolution and contact line migration, respectively. In isotropic case, by adding a small surface diffusion regularization for the contact line migration, we could apply the parametric finite element methods to solve both the surface evolution and plane curve evolution. Furthermore, the parametric finite element method is generalised to the weakly anisotropic case.

Finally, the sharp interface model is extended to the cases when the surface energy is strongly anisotropic and when the substrate is curved. Besides, we study the migration of the toroidal thin films under the axis-symmetry, and a reduced model to describe the migration rate is obtained via the Onsager’s principle.
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2D two dimensions
3D three dimensions
$\mathbb{R}^d$ d dimensional Euclidean space
PFEM parametric finite element method
$\Omega_0$ atomic volume
$D_s$ surface diffusivity
$\nu$ the number of diffusing atoms per unit area
$k_B T_e$ thermal energy
$\gamma_0$ unit scale of film/vapor interfacial energy density
$L$ length scale
$\gamma_{FS}$ film/substrate interfacial energy density
$\gamma_{VS}$ vapor/substrate interfacial energy density
$\sigma$ a dimensionless parameter equals to $\frac{\gamma_{VS} - \gamma_{FS}}{\gamma_0}$
$\epsilon$ small perturbation parameter
$\delta$ small regularization parameter
$t$ time
$s$ arc length of the film/vapor interface
$\rho$ a variable for parameterizing the film/vapor interface
\begin{itemize}
  \item $S$: surface
  \item $S_{\text{sub}}$: substrate
  \item $n$: outer unit normal vector
  \item $n_{\text{sub}}$: outer unit normal vector of $\Gamma$ on substrate
  \item $c_{\Gamma}$: unit co-normal vector on boundary $\Gamma$
  \item $c_{\Gamma}^\gamma$: anisotropic co-normal vector
  \item $n_{\text{sub}}$: unit normal vector of the substrate
  \item $\kappa$: curvature of curve
  \item $\mathcal{H}$: mean curvature
  \item $\mathcal{K}$: Gaussian curvature
  \item $M_x(\phi)$: rotational matrix along $x$ axis with angle $\phi$ under right hand rule
  \item $M_y(\phi)$: rotational matrix along $y$ axis with angle $\phi$ under right hand rule
  \item $M_z(\phi)$: rotational matrix along $z$ axis with angle $\phi$ under right hand rule
  \item $S^2$: the surface of unit sphere
  \item $X(\cdot,t)$: local parametrization of the film/vapor interface
  \item $X_{\Gamma}(\cdot,t)$: local parametrization of the contact line
  \item $W$: total interfacial (surface) energy
  \item $W_{\text{FV}}$: film/vapor interfacial energy
  \item $W_{\text{FS}}$: film/substrate interfacial energy
  \item $W_{\text{VS}}$: vapor/substrate interfacial energy
  \item $W_{\text{int}}$: interfacial energy
  \item $W_{\text{sub}}$: substrate energy
  \item $\gamma(n)$: surface energy density
  \item $\gamma(\theta,\phi)$: surface energy density in spherical coordinates
  \item $\hat{\gamma}(n)$: homogeneous extension of $\gamma$
  \item $\xi$: Cahn-Hoffman vector
\end{itemize}
H₂\text{γ} \quad \text{Hessian matrix of } \hat{\gamma}

T_ε \quad \text{geometric transformation}

V \quad \text{variation vector field}

\dot{\phi}(Ω; V) \quad \text{material derivative}

\phi'(Ω; V) \quad \text{shape derivative}

dF(Ω; V) \quad \text{first variation in direction } V

\psi(t) \quad \text{Mesh-distribution function}

\mathcal{T}_xS \quad \text{tangent space to surface } S \text{ at point } x

\mathcal{N}_xS \quad \text{normal space to surface } S \text{ at point } x

\mathcal{F} \quad \text{Frank shape}

\mathcal{W} \quad \text{Wulff shape}

\perp \quad \text{rotating vector by 90 degrees in the clockwise direction}

\nabla_s \quad \text{surface gradient operator}

\Delta_s \quad \text{Laplace-Beltrami operator}

\times \quad \text{cross product}
Introduction

1.1 Interface/surface Dynamics

1.1.1 Physics background

Interfacial problems are typical in material science for fluid or solid systems and have been widely studied in different aspects. A drop of water on a leaf or a soap bubble tend to form near-spherical shape, as the sphere has the smallest surface area to volume ratio. This phenomenon, know as surface tension, results form the cohesive forces among the liquid molecules. More precisely, molecules inside the liquid are pulling equally in every direction by their neighbouring liquid molecules. However, the molecules that wander to the surface will lose part of their cohesive interactions from outside. Therefore, these molecules are pulled inwards and the force the liquids to adjust their shapes such that the number of molecules on the surface must be minimized. The minimization of the number of molecules on the surface results in a minimization of the surface area, thus giving the spherical shape.

Several effects of the surface tension can be observed with the ordinary water in our daily life, such as the beading of rain water on a leaf, the water dripping from a tap. Although surface tension occurs on solid surface as well, yet few corresponding effects of surface tension in solids has been observed in daily life. The is due to that...
the mechanism for solid surface is much more complicated than that of the fluid interface. Different mechanisms are competing among each other to determine the shape evolution for solid surface. In micro and nano-scale, surface tension could be the dominant dynamics for solid surface.

Surface tension of a liquid, usually represented by $\gamma$, can be viewed as a force per unit length or energy per unit area. The system is trying to find a state such that the surface energy is minimized.

### 1.1.2 Interfacial energy density

Unlike liquid or amorphous solids, the interface energy for many materials could be various for different crystallographic orientations, and this anisotropy in the surface energy could lead faceting for crystals. Therefore, for anisotropic materials, as most theories start with, the surface energy density, denoted by $\gamma$, is assumed to be dependent on the direction $\mathbf{n}$, the oriented normal of the interface. More precisely, the interfacial energy density can be expressed as a function defined on the surface of a unit sphere denoted by $S^2$:

$$\gamma(\mathbf{n}) : S^2 \to \mathbb{R}, \quad (1.1.1)$$

where $\mathbf{n}$ is the unit normal vector of the interface. Although there are cases when the interface energy density depends on the temperature, position, curvature [61, 104, 106] and so on, for simplicity, here we only restrict to the case when the interface energy density is dependent on the orientation.

When $\gamma(\mathbf{n})$ is smooth, many theories indicate that the derivatives of $\gamma(\mathbf{n})$ play an important role in studying the dynamics and equilibrium problems for the crystals evolutions. However, calculating the derivative with respect to $\mathbf{n}$ restricts us on the surface of a unit sphere, which could cause a lot of troubles. For convenience and further discussion, we usually extend the domain of $\gamma$ from $S^2$ to the whole $\mathbb{R}^3$ homogeneously [34] in the following

$$\hat{\gamma}(\mathbf{p}) = |\mathbf{p}|\gamma(\frac{\mathbf{p}}{|\mathbf{p}|}), \quad \forall \mathbf{p} \in \mathbb{R}^3 \setminus \{0\}. \quad (1.1.2)$$
Under this extension, $\hat{\gamma}$ satisfies the following equation

$$\hat{\gamma}(\lambda \mathbf{p}) = |\lambda| \hat{\gamma}(\mathbf{p}), \quad \forall \lambda \neq 0, \; \mathbf{p} \in \mathbb{R}^3 \setminus \{\mathbf{0}\}. \quad (1.1.3)$$

Moreover, if $\hat{\gamma}(\mathbf{p}) \in C^2(\mathbb{R}^3)$, we have

$$\nabla \hat{\gamma}(\mathbf{p}) \cdot \mathbf{p} = \hat{\gamma}(\mathbf{p}), \quad \nabla \hat{\gamma}(\lambda \mathbf{p}) = \text{sign}(\lambda) \nabla \hat{\gamma}(\mathbf{p}),$$

$$H_{\gamma}(\mathbf{p}) \mathbf{p} \cdot \mathbf{q} = 0, \quad H_{\gamma}(\lambda \mathbf{p}) = \frac{1}{|\lambda|} H_{\gamma}(\mathbf{p}), \quad \forall \mathbf{p}, \mathbf{q} \in \mathbb{R}^3 \setminus \{\mathbf{0}\}, \lambda \neq 0. \quad (1.1.4)$$

Here $\nabla \hat{\gamma}$ denotes the gradient of $\hat{\gamma}$ and $H_{\gamma}$ represents the Hessian of $\hat{\gamma}$. It is easy to show that the matrix $H_{\gamma}$ is symmetric and has a zero eigenvalue: $H_{\gamma}(\mathbf{p}) \mathbf{p} = \mathbf{0}$.

Here are some examples of some choices of the anisotropy:

- **Isotropic surface energy**
  $$\gamma(\mathbf{n}) = |\mathbf{n}| = 1. \quad (1.1.5)$$

- **Cubic surface energy**
  $$\gamma(\mathbf{n}) = 1 + a[n_1^4 + n_2^4 + n_3^4]. \quad (1.1.6)$$

- **Ellipsoidal surface energy**
  $$\gamma(\mathbf{n}) = \sqrt{a_1^2 n_1^2 + a_2^2 n_2^2 + a_3^2 n_3^2}. \quad (1.1.7)$$

- **Facet/cusp surface energy**
  $$\gamma(\mathbf{n}) = |n_1| + |n_2| + |n_3|. \quad (1.1.8)$$

The simplest case is the isotropic case when $\gamma(\mathbf{n})$ is a constant. Some other anisotropies are given such as the cubic crystalline surface energy (Eq. (1.1.6)) and ellipsoidal surface energy (Eq. (1.1.7)). In application of materials science, the surface energy is usually piecewise smooth and has some “cusped” points, where it is not differentiable [61,89]. A typical example for this type anisotropy is given in Eq. (1.1.6). We can regularize the energy as following to ensure the smoothness.

$$\gamma(\mathbf{n}) = \sqrt{\varepsilon^2 + (1 - \varepsilon^2)n_1^2} + \sqrt{\varepsilon^2 + (1 - \varepsilon^2)n_2^2} + \sqrt{\varepsilon^2 + (1 - \varepsilon^2)n_3^2}. \quad (1.1.9)$$
1.1 Interface/surface Dynamics

The classification of anisotropies can be different due to different criteria. In mathematics, we usually classify the anisotropies into two categories by checking whether the following inequality is satisfied:

\[ H_\gamma(p)q \cdot q \geq \lambda_0, \quad \forall q \cdot p = 0, \quad q, p \in S^2. \]  

(1.1.10)

Here \( \lambda_0 \) is a positive constant to be found. If the anisotropy satisfies Eq. (1.1.10), we call it weak anisotropy. Otherwise, we call it strong anisotropy. Eq. (1.1.10), also called convexity condition, is crucial to the stability of the Wulff shape [122], well-posedness of the surface diffusion flow [67] and numerical analysis [34]. In materials science, some people may classify the facet anisotropy with cusps as strong anisotropy [71]. The classification criteria could be better understood in two dimensions where the anisotropy is given as \( \gamma(\theta) \). Here \( \theta \) satisfies \( n = (-\sin \theta, \cos \theta)^T \), \( \tau = (\cos \theta, \sin \theta)^T \), we can easily obtain that

\[ H_\gamma(n) = (\gamma(\theta) + \gamma''(\theta)) \begin{pmatrix} n_2^2 & -n_1n_2 \\ -n_1n_2 & n_1^2 \end{pmatrix}. \]  

(1.1.11)

Thus we have \( H_\gamma(n) \tau \cdot \tau = \gamma(\theta) + \gamma''(\theta) \). This indicates that Eq. (1.1.10) is related to the surface stiffness \( \gamma(\theta) + \gamma''(\theta) \). In three dimensions, \( H_\gamma(n) \tau \cdot \tau \) can be regarded as the surface stiffness in the \( \tau \) direction.

Usually the anisotropy function \( \gamma(n) \) can be geometrically represented by the radial plot of \( \gamma \), and we call it \( \gamma \)-plot. The shape can be expressed as

\[ F = \{ x \in \mathbb{R}^3 : |x| \leq \gamma(\frac{x}{|x|}) \}. \]  

(1.1.12)

### 1.1.3 Cahn-Hoffman \( \xi \)-vector

Cahn and Hoffman developed the theory of Cahn-Hoffman \( \xi \)-vector [27, 65] to describe the surface energies density instead of using the traditional scalar function \( \gamma \) or \( \gamma \)-plot. It is mathematically defined as

\[ \xi(n) = \nabla(r\gamma) = \nabla \gamma(n), \text{ with } \xi_j(n) = \frac{\partial \gamma}{\partial p_j}(n) \text{ where } j = 1, 2, 3. \]  

(1.1.13)
If the surface energy density is given in terms of the spherical coordinates, $\gamma(\theta, \phi)$, with $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$, under the homogeneous extension, we have

$$\dot{\gamma}(p) = |p| \gamma \left( \tan^{-1} \left( \frac{\sqrt{p_1^2 + p_2^2}}{p_3} \right), \tan^{-1} \left( \frac{p_2}{p_1} \right) \right).$$

(1.1.14)

Thus the Cahn-Hoffman $\xi$-vector can be written as

$$\xi(n) = \nabla \dot{\gamma}(n) = \gamma n + \gamma n \theta + \frac{1}{\sin \theta} \gamma n \phi,$$

(1.1.15)

where in this expressions,

$$n = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)^T,$$

(1.1.16a)

$$\theta = (\cos \theta \cos \phi, \cos \theta \sin \phi, -\sin \theta)^T,$$

(1.1.16b)

$$\phi = (-\sin \phi, \cos \phi, 0)^T.$$

(1.1.16c)

This vector consists of the normal component and tangential component, with each part representing the tendency of minimizing the surface energies by contraction or rotation respectively [65].

### 1.1.4 Surface energy and evolution

Given the surface energy density $\gamma(n)$, the total surface energy is a integration over the interface $S$,

$$W = \iint_S \gamma(n) \, dS.$$  

(1.1.17)

In polycrystalline material, the grain boundary migrations are driven by curvature, where a grain boundary move with a velocity that is proportional to its mean curvature [108]. This motion is called mean curvature flow and can be regarded as the $L^2$ gradient flow of the surface energy. Under the mean curvature flow, the surface with isotropic surface energy will evolve into a spherical shape and shrink inward uniformly.

Another important kinetic for surface evolution is surface diffusion flow [86], which can be regarded as the $H^{-1}$ gradient flow of the surface energy. This geometric flow forces the surface to reduce the surface energy while fixing the enclosed volume as a constant.
1.2 Solid State Dewetting

Figure 1.1: Solid thin films dewet to from isolated islands, the image is taken from [117].

1.2.1 Physical experiments and applications

Solid thin film on the substrate is typically unstable and can dewet or agglomerate to form isolated islands (see Fig. 1.1) when heated to sufficiently high temperature, but well below the material’s melting point [117]. During this process, the thin film remains in the solid state, thus it is called solid-state dewetting. Driven by capillarity, solid-state dewetting is a process moving towards the equilibrium by minimizing the total surface energy.

In recent physical experiments, some morphological features were observed in the intermediate state of solid-state dewetting. These features include edge retraction, rim growth, hole formation and growth and so on.

For solid-state dewetting, materials from the triple line (where the film, vapor and substrate meet) and corner will be transported to the flat area. This mass transport leads to the formation of rim and valley at edges. See Fig. 1.2(g), as the edge retracts, the rim grows and the depth of the valley increases. For small patches, the valley finally disappears. However, when the size of the patches is large enough, the valley will reach the substrate before they merge and form hole (see Fig. 1.2(e),(f)) or edge pinch-off. Moreover, the finger instability can be observed
Figure 1.2: Dewetting of Ni with different initial sizes. (e)-(h) shows the corresponding height profile of the single thin film. The image is taken from [128].

during the edge retraction [33, 50, 68, 69, 77]. The thin film produces protruding fingers at the edge by forming rims with different heights and triple lines at different positions, see Fig. 1.3. Anisotropy can greatly influence the morphologies evolution of thin film by producing the faceting geometry. When there exist surfaces parallel

Figure 1.3: The left image taken from [68] shows the finger instability during dewetting. The right image taken from [70] shows the corner instability.
to the substrate, and the orientations of these surfaces do not take a minimum for the surface energy density, the thin film may develop a wave along the flat surface during the edge retraction. This morphological evolution is called the faceting instability. Corner instability is another morphological characteristic for solid-state dewetting. Anisotropic thin films can dewet to form polygonal shaped holes, and these holes can grow anisotropically with increasing annealing time. Physical experiments demonstrate that corners retract faster than the centre of the edges, thus causing dendritic or star-shaped holes [2,139].

![Faceting instability for long retracting edges. This image is taken from [130].](image)

In summary, the morphologies evolution of thin film could be affected by many parameters.

- Thin film geometry: experiments by Ye and Thompson [128,129] has shown the geometry of the thin film, including the size, orientation, location of holes and so on, could dramatically influence the shape evolution (see Fig. 1.5 for an example).

- Substrate topology: the morphological evolution of the thin film could be greatly influenced by the topology of the substrate [53, 83, 90, 112]. It shows that ordered topologically substrate produces ordered dewetting structures.
1.2 Solid State Dewetting

Figure 1.5: Dewetting of cross patches with pre-patterned internal circular holes. The initial size of the patches and the size and location of holes are different. This image is taken from [129].

- Anisotropic surface energies: the anisotropy of the surface energies produces faceting geometry for the thin film and also influences the morphological evolution of the thin film [127–130].

- Some other parameters such as the temperature, or outer environment and so on.

Solid thin films are fundamental components of the microelectronic and optoelectronic devices. The morphological evolution of the small thin film could be a great issue and should be prevented in order to keep the reliability of the device. Thus many research has been carried out to characterize and suppress dewetting in this microsystem. However, the recent understanding of solid-state dewetting makes it possible to provide positive influence. For example, it can be purposely induced to produce catalysts for growth of carbon nanotubes and semiconductor nanowires.
The wide applications of solid-state dewetting make it urgent to have a better understanding of the kinetic patterns and features of solid-state dewetting.

### 1.2.2 Interfacial energies and surface diffusion

![Diagram of a solid thin film on a flat rigid substrate in three dimensions.](image)

Figure 1.6: A schematical illustration of a solid thin film on a flat rigid substrate in three dimensions.

Fig. 1.6 is a schematic illustration of a solid thin film on a flat rigid substrate in three dimensions. The total surface energy of the solid-state dewetting, can be expressed in the following

\[
W = \int_{S_{FV}} \gamma_{FV} \ dS_{FV} + \int_{S_{FS}} \gamma_{FS} \ dS_{FS} + \int_{S_{VS}} \gamma_{VS} \ dS_{VS} \ .
\] (1.2.1)

In these expressions, \(S_{FV}\), \(S_{FS}\) and \(S_{VS}\) represent the film/vapor, film/substrate and vapor/substrate interfaces. Here \(\gamma\) with the subscripts denote the corresponding surface energy density respectively. The total surface energy includes the film/vapor interface energies and substrate energies. Assume \(\gamma_{FS}, \gamma_{VS}\) are constants, while \(\gamma_{FV} = \gamma(n)\), choose a bounded domain with dimensions \(L_x \times L_y\) on the substrate,
then the total surface energy of the bounded system is given as
\[
W = \int_S \gamma_F V dS_F + \int_{S_{FS}} \gamma_{FS} dS_{FS} + \int_{S_{VS}} \gamma_{VS} dS_{VS}
\]
\[
= \int_S \gamma(n) dS + A(\Gamma)\gamma_{FS} + (L_x L_y - A(\Gamma))\gamma_{VS}
\]
\[
= \int_S \gamma(n) dS + (\gamma_{FS} - \gamma_{VS})A(\Gamma) + L_x L_y \gamma_{VS}.
\]
(1.2.2)

Here \( \Gamma \) is the contact line and \( A(\Gamma) \) represents the area enclosed by \( \Gamma \) on the substrate. Since the term \( L_x L_y \gamma_{VS} \) is fixed as a constant, thus we can always omit it and simplify the total energy as
\[
W = \int_S \gamma(n) dS + (\gamma_{FS} - \gamma_{VS})A(\Gamma).
\]
(1.2.3)

Unlike liquid dewetting, surface diffusion is the dominant mass transport and plays the essential role in determining the shape evolution of solid thin films compared to other types of transport process: viscous flow, evaporation/condensation, and volume diffusion. The surface normal velocity governed by surface diffusion for isotropic materials (\( \gamma = \gamma_0 \) is a constant) can be mathematically described by Mullins \[86\] in the following
\[
v_n = B \nabla^2 \mathcal{H}, \quad \text{with} \quad B = \frac{D_s \gamma \Omega^2 \nu}{K_B T_e}.
\]
(1.2.4)

Here \( D_s \) is the surface diffusivity, \( k_B T_e \) is the thermal energy, \( \Omega_0 \) represents the atomic volume, \( \nu \) is the surface concentration of mobile atoms, \( \mathcal{H} \) is the mean curvature of the surface. \( \nabla_s \) is the surface gradient operator. In his derivation, the chemical potential is given as
\[
\mu = \Omega_0 \mathcal{H}.
\]
(1.2.5)

Then by the Fick’s first law, the flux of the surface atoms is given by
\[
J = -\frac{D_s \nu}{K_B T_e} \nabla_s \mu.
\]
(1.2.6)

The normal velocity of the surface is given by multiplication of \( \Omega_0 \) and the surface divergence of \(-J\) \[4\],
\[
v_n = -\Omega_0 \nabla_s \cdot J = \frac{D_s \gamma \Omega^2 \nu}{K_B T_e} \nabla^2 \mathcal{H}.
\]
(1.2.7)
The surface diffusion flow, governed by fourth order geometric equations, was analytically investigated for the existence in two dimensions [47, 54, 93]. They showed the local existence, regularity and uniqueness of the solution for an initial smooth curve and global existence for small perturbation of circles. Moreover, Escher et.al [48] extended the theories to the three-dimensional hypersurfaces.

One of the fundamental properties for surface diffusion flow is the conservation of the volume enclosed by the closed curves or surfaces. Besides, the arc length of the closed curves or area of the closed surfaces is decreasing under the surface diffusion flow. Actually, motion by surface diffusion can be regarded as the $H^{-1}$ gradient flow for the energy functional [29]. Eq. (1.2.4) can be extended to the anisotropic case by replacing the mean curvature $H$ with weighted mean curvature $H_\gamma$ [115], which is defined as

$$H_\gamma = \nabla_s \cdot \xi,$$

with $\xi$ denoting the Cahn-Hoffman vector.

### 1.2.3 Contact line migration

In solid-state dewetting, the intersection of the thin film, vapor and substrate produces contact line, see Fig. 1.6. Thus the migration for the contact line becomes an additional kinetic feature for solid-state dewetting, in addition to the surface diffusion flow.

When two immiscible fluids are placed on a solid substrate, the intersection of the two fluid phases with the substrate forms a contact line. The moving contact line problems for fluid mechanics have been widely studied in recent years [7, 37, 96–98, 100–103, 119]. In polycrystalline materials, similar problems have also been discussed and studied in grain boundary systems for the migration of triple lines or junctions [32, 55, 56, 82, 95, 118, 134].

For solid-state dewetting with isotropic surface energy, the equilibrium configuration for the static contact line is the same as that in fluid mechanics or grain
boundaries, where the equilibrium contact angle (see Fig. 1.7) is described by the Young-Dupree equation \[131\]

\[
\gamma_{VS} = \gamma_{FS} + \gamma_{FV} \cos \theta_c.
\] (1.2.9)

Here \(\theta_c\) is the static contact angle on the contact line. The static contact line condition (Eq. (1.2.9)) has been widely adopted as the boundary condition for the dynamic sharp interface model \[41, 111, 125\]. The static contact line condition can be extended to the anisotropic case in two dimensions \[9, 120\]

\[
\gamma_{VS} = \gamma_{FS} + \gamma(\theta_c) \cos \theta_c - \gamma'(\theta_c) \sin \theta_c,
\] (1.2.10)

where \(\gamma_{FV} = \gamma(\theta)\) with \(\theta\) representing the angle made by the normal vector of the interface with respect to the +y direction. Similar static boundary conditions for the contact line have also been proposed for phase field model \[46, 66\].

When the static contact line condition is coupled as the boundary condition for the dynamic model, the contact angle is assumed to be fixed at its equilibrium value during the evolution. This assumption is reasonable when the thin film approaches the equilibrium shape. However, experimental and atomistic simulations for fluid
mechanics and grain boundary migrations \cite{55, 56, 82, 95, 100, 102, 118} demonstrate that the contact angle need not be in equilibrium. This deviation from the equilibrium angle could be explained by considering the atomic structure of the contact line itself. A finite mobility of the contact line implies this deviation, while infinite mobility implies that the contact angle is always at its equilibrium value. Thus, instead of treating the static contact line condition as a boundary condition, the contact line mobility was introduced recently with a relaxation kinetic (see Eq. (1.4.2b) and Eq. (1.4.2c)) for the contact point positions in two dimensions \cite{67, 120}. Some other treatments for the motion of the contact line have been presented by Dornel \textit{et al.} \cite{40} and Klinger \textit{et al.} \cite{72, 73}.

1.3 Equilibrium shapes

The equilibrium shape of solid-state dewetting is the minimization of the total surface energy while fixing the total volume of the thin film. The problem is mathematically expressed in the following

$$\min_{\Omega} \left( \int_{\Gamma} \gamma(n) dS + (\gamma_{FS} - \gamma_{VS})A(\Gamma) \right) \quad \text{s.t.} \quad |\Omega| = \text{const.}$$ \hfill (1.3.1)

Here $\Omega$ is the region enclosed by the film/vapor interface and substrate. If the thin film is free standing and isolated, then the contribution to the total surface energy is only the film/vapor surface energy. In other words, $S$ is a closed surface, and the minimization problem can be reduced to

$$\min_{\Omega} \left( \int_{S} \gamma(n) dS \right) \quad \text{s.t.} \quad |\Omega| = \text{const.}$$ \hfill (1.3.2)

1.3.1 Wulff construction

After Gibbs first proposed the equilibrium problem Eq. (1.3.2), Wulff presented a theory, known as Gibbs-Wulff theorem, for the equilibrium shape without proof in 1901 \cite{126}. In the theory, he stated that the distance from the centre of the crystal shape to the face is proportional to the surface energy density of that face. Later,
Figure 1.8: The Wulff construction for two-dimensional examples, where (a) $\gamma(n) = 1 + 0.2(n_1^2 + n_2^2 - 6n_1^2n_2^2)$, (b) $\gamma(n) = |n_1| + |n_2|$. The blue line represents the $\gamma$-plot and all the black lines represent the lines that perpendicular to $n$.

subsequent proofs of this theorem have been presented in many works [26, 38, 61, 62, 75, 81].

The equilibrium shape of the crystal can be geometrically constructed based on the $\gamma$-plot, and the finally obtained shape is called Wulff shape denoted by $\mathcal{W}$. The procedure can be stated as following four steps:

1. Carry out the polar plot of $\gamma(n)$ and obtain the $\gamma$-plot.

2. For each direction $n$, draw a plane perpendicular to $n$ with distance to the origin equaling to $\gamma(n)$.

3. The plane draw from the step 2 divides the space into two regions, and the region which is far from the origin is discarded.

4. When this has been done in all directions, the remaining convex region is called the Wulff shape.

Fig. 1.8, is a schematic illustration of the Wulff construction in two dimensions for
two anisotropies. In Fig. 1.8(b), $\gamma(n)$ is chosen as cusp/facet surface energy density $\gamma(n) = |n_1| + |n_2|$. As a consequence, the corresponding Wulff shape consists of sharp corners and flat edges. Here $\gamma(n)$ is not differentiable where $n_1, n_2$ are changing their signs, which demonstrates that Wulff construction does not require the continuity and smoothness of $\gamma(n)$. Moreover, as can be seen from Fig. 1.8(a), the equilibrium shape obtained via Wulff construction has some missing orientations on the corners. This indicates that Wulff construction can be interpreted as a convexification of the $\gamma$-plot by removing all the unstable orientations. Herring presented a geometric criteria for occurrence of the missing orientation in the Wulff shape via Herring sphere construction [61], see Fig. 1.9. The construction is based on the $\gamma$-plot and can be stated as following:

1. Carry out the polar plot of $\gamma(n)$ and obtain the $\gamma$-plot.

2. For any orientation $n$, construct a sphere that is tangent to the $\gamma$-plot at $\gamma(n)$ and passing through the origin.

3. If the sphere is totally inside the $\gamma$-plot, then orientation $n$ appears on the equilibrium shape. Otherwise it is missing on the equilibrium shape.

Figure 1.9: (a) A schematic illustration of Herring sphere construction. (b) $1/\gamma$-plot. Both figures are taken from [105].
If the tangent sphere is totally inside the $\gamma$-plot, it is equivalent to that the plane inverted from the sphere is totally outside the $1/\gamma$-plot. Thus the non-convexity of the $1/\gamma$-plot can also be used to test the occurrence of the missing orientation [105].

The Wulff shape and the Frank shape ($1/\gamma$-plot) can be mathematically expressed as

$$W = \{ x \in \mathbb{R}^3 : x \cdot n \leq \gamma(n), \quad \forall n \in S^2 \}. \quad (1.3.3a)$$

$$F = \{ x \in \mathbb{R}^3 : \gamma(\frac{x}{|x|}) \leq 1 \}. \quad (1.3.3b)$$

As the magnitude of the normal component of $\xi$ equals $\gamma(n)$ (see Eq. (1.1.15)), in view of the construction procedure of the Wulff shape, it is easy to know $\xi$-plot shares similar geometry to the Wulff shape [65, 89]. Precisely speaking, the $\xi$-plot is the mathematical representation of the boundary of the Wulff shape when no missing orientation occurs on the Wulff shape. On the other hand, when certain orientations are missing on the Wulff shape, the corresponding $\xi$-plot will have ears and needed to be truncated in order to obtain the equilibrium shape. As depicted in Fig. 1.11, it shows the $\gamma$-plot, $1/\gamma$-plot and $\xi$-plot for the cubic surface energy with different choices of the degree of anisotropy. When $a = 0.3$, the corresponding $1/\gamma$-plot is convex and the $\xi$-plot is directly the boundary of the Wulff shape. When $a = 1.0$, the anisotropy becomes strong, $1/\gamma$-plot is no longer convex and the $\xi$-plot forms some ears. We can summarise above results in Table. 1.1,

### 1.3.2 Winterbottom construction

Thin films are not always free standing and can be attached to a substrate. The Wulff construction is not able to obtain the equilibrium shape which minimizes the total surface energy in this case since the additional substrate energy should be included, see Eq. (1.3.1). Based on the thermodynamic approach, Winterbottom [123] derived that the equilibrium shape of problem defined in Eq. (1.3.1) is directly
1.3 Equilibrium shapes

Figure 1.10: $\gamma$-plot, $1/\gamma$-plot and $\xi$-plot for different anisotropies. (a) Isotropic surface energy $\gamma(n) = 1$; (b) cubic anisotropic surface energy defined as $\gamma(n) = 1 + a(n_1^4 + n_2^4 + n_3^4)$ with $a = 0.3$; (c) ellipsoidal surface energy $\gamma(n) = \sqrt{a_1 n_1^2 + a_2 n_2^2 + a_3 n_3^2}$ with $a_1 = 4, a_2 = a_3 = 1$; (d) facet/cusp surface energy defined as $\gamma(n) = |n_1| + |n_2| + |n_3|$ with smooth regularization in Eq. (1.1.9).
1.3 Equilibrium shapes

Table 1.1: Some distinguished properties between the strong anisotropy and weak anisotropy for $\gamma(n)$

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<thead>
<tr>
<th>$\gamma(n)$</th>
<th>Weak anisotropy</th>
<th>Strong anisotropy</th>
</tr>
</thead>
<tbody>
<tr>
<td>$W$ (Wulff shape)</td>
<td>no missing orientation</td>
<td>missing orientation exists</td>
</tr>
<tr>
<td>$F(1/\gamma$-plot)</td>
<td>convex</td>
<td>not convex</td>
</tr>
<tr>
<td>$\xi$-plot</td>
<td>no ears</td>
<td>forming ears</td>
</tr>
<tr>
<td>Math criteria</td>
<td>$(H_\gamma(n) \tau) \cdot \tau &gt; 0$</td>
<td>$(H_\gamma(n) \tau) \cdot \tau &lt; 0$, for some $\tau$</td>
</tr>
</tbody>
</table>

Figure 1.11: The $\gamma$-plot, $1/\gamma$-plot and $\xi$-plot are shown in column 1,2,3 respectively. The first row is for weak anisotropy: $\gamma(n) = 1 + 0.3(n_1^4 + n_2^4 + n_3^4)$ and the second row is for strong anisotropy: $\gamma(n) = 1 + (n_1^4 + n_2^4 + n_3^4)$. 
the Wulff shape of a general surface tension $\gamma^*$, which is defined as

$$\gamma^*(\mathbf{n}) = \begin{cases} 
\gamma(\mathbf{n}), & \mathbf{n} \text{ corresponds to the film/vapor interface,} \\
\gamma_{FS} - \gamma_{VS}, & \text{otherwise.}
\end{cases} \quad (1.3.4)$$

Thus the equilibrium shape for problem Eq. (1.3.1) can be obtained by cutting the Wulff shape of $\gamma(\mathbf{n})$ with the plane $z = \gamma_{VS} - \gamma_{FS}$.

### 1.4 Models and computational methods

The first sharp interface model for solid-state dewetting was proposed by Srolovitz and Safran [111] to investigate the hole growth under the assumption of isotropic surface energy and cylindrical symmetry. See Fig. 1.12, if the thin film profile is represented by $(r, h(r))$, in the small slop limit ($\frac{\partial h}{\partial r} \ll 1$), the surface diffusion equation will reduce to

$$\frac{\partial h}{\partial t} = -\frac{B}{r} \frac{\partial}{\partial r} \left[ r \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial h}{\partial r} \right) \right) \right], \quad r > \rho, \ t > 0, \quad (1.4.1)$$
with \( B = \frac{D_{st} \gamma_F \Omega^2}{k_B T_e} \). For the contact points, the following boundary conditions were included

\[
\begin{align*}
    h(\rho, t) &= -a, \quad (1.4.2a) \\
    \frac{\partial h}{\partial r}(\rho, t) &= \tan \theta_c, \quad (1.4.2b) \\
    \frac{\partial^3 h}{\partial r^3}(\rho, t) + \frac{1}{\rho} \frac{\partial^2 h}{\partial t^2}(\rho, t) - \frac{1}{\rho^2} \frac{\partial h}{\partial r}(\rho, t) &= 0, \quad (1.4.2c) \\
    \lim_{r \to \infty} h(r, 0) &= 0. \quad (1.4.2d)
\end{align*}
\]

The boundary conditions Eq. (1.4.2a) and Eq. (1.4.2d) come directly from the coordinate system. Eq. (1.4.2b) expresses the equilibrium contact angle at the boundary while Eq. (1.4.2c) implies there is no source or sink for matter at the contact point. Based on this model, they showed that large holes can migrate such that the edge retraction distance can be scaled by \( t^{1/4} \) while small holes will shrink.

This model was then generalized to both the two-dimensional case [125] and three-dimensional case with cylindrical symmetry [42] in Lagrangian representation. Numerical results in [125] demonstrated that semi-infinite thin film undergoes a periodic mass shedding. Moreover, the authors showed numerically and analytically that the edge retraction distance could be scaled by \( t^{2/5} \) at a later time for the semi-infinite film.

However, these models all start from the initial assumption that the surface energy is isotropic, thus the influence of the crystalline anisotropy on the morphological evolution for solid-state dewetting could be ignored. Besides, physical experiments [2, 127, 130, 139] have demonstrated that surface energy anisotropy could greatly influence the kinetics of solid-state dewetting, such as the faceting instability and corner instability. To include this crystalline anisotropy, recently some new models have been proposed, including the discrete model by Dornel [40], a kinetic Monte Carlo method [43, 92, 92] and the crystalline method [70, 138]. Some other models have been presented to study kinetics of hole growth [2, 139]. While the drawback of these approaches is that the evolution does not account for the full
anisotropic free energy of the system or do not represent a completely mathematical description.

Figure 1.13: A schematic illustration of a solid thin film on a flat rigid substrate in two dimensions, this image is taken from [120].

More recently, based on thermodynamic variation, Wang et al. [120] derived rigorously a continuum sharp interface model for simulating the solid-state dewetting with weakly anisotropic surface energies. In their model, see Fig. 1.13, they assume the moving film/vapor interface is given by an open curve \( X(x(s,t), y(s,t)) \), where \( s \) is the arc length and \( t \) is time. Then the dimensionless sharp interface model with weakly anisotropic surface energies in two dimensions can be described as

\[
\frac{\partial X}{\partial t} = \frac{\partial^2}{\partial s^2} \left[ \left( \gamma(\theta) + \gamma''(\theta) \right) \kappa \right] n. \tag{1.4.3}
\]

They also proposed the following boundary conditions

\[
y(x_c^l, t) = y(x_c^r, t) = 0, \tag{1.4.4a}
\]

\[
\frac{dx_c^l}{dt} = \eta \left( \gamma(\theta_d^l) \cos \theta_d^l - \gamma'/(\theta_d^l) \right) \sin \theta_d^l - \sigma, \tag{1.4.4b}
\]

\[
\frac{dx_c^r}{dt} = -\eta \left( \gamma(\theta_d^r) \cos \theta_d^r - \gamma'/(\theta_d^r) \right) \sin \theta_d^r - \sigma, \tag{1.4.4c}
\]

\[
\frac{\partial \mu}{\partial s} (x_c^l, t) = \frac{\partial \mu}{\partial s} (x_c^r, t) = 0. \tag{1.4.4d}
\]
1.4 Models and computational methods

They introduced the relaxation kinetics Eqs. (1.4.4b),(1.4.4c) for the contact point position to replace the static contact angle equation Eq. (1.4.2b). The governing equations of the models belong to a new type of 4th-order geometric evolution partial differential equations about open curve interface tracking problems, which include anisotropic surface diffusion flow and contact line migration. With Willmore energy regularization, this model was then generalized to the strongly anisotropic case [67]. Besides, a new zero-curvature boundary condition was included to ensure the energy dissipation and wellposedness for the new 6th-order PDEs.

There is a long history in the numerical simulations of moving interfacial problems, and different numerical methods have been proposed in the literature for simulating the evolution of a closed curve/surface under mean curvature flow, surface diffusion flow, Willmore flow and so on. Some theories on the stable finite element method based on the graph representation of the surface [5,34–36] were well developed, and corresponding error analysis was derived. However, the condition that the evolution surface can be explicitly parameterized on some base domain in $\mathbb{R}^n$ is so harsh to satisfy in most cases. Numerical methods that could be applied to more general curves/surfaces became more popular, such as the marker-particle methods [63,78,79], and the parametric finite element methods [6,58,94]. Among these methods, the main issue is that mesh quality during the curve/surface evolution could not be preserved and can deteriorate to make the scheme unstable; thus these algorithms need some kinds of mesh regularizations or re-meshing to maintain the mesh quality. Recently, this mesh issue has been well overcome by J.W. Barrett et al. [16,17,19,20] with a new novel parametric finite element method, which has very good properties with respect to the distribution of the mesh points. Precisely, this scheme introduced a particular tangential motion for the mesh points such that these mesh points automatically moved tangentially over the surface and maintained good mesh properties. Therefore the discrete scheme can be performed without any mesh regularization. More recently, this scheme has been extended for simulating the grain boundary motion and application of thermal grooving and sintering [24,134].
1.4 Models and computational methods

For solid-state dewetting, i.e., the evolution of an open curve/surface under surface diffusion flow and contact line migration, based on the previous mathematical models and numerical simulations, different numerical algorithms have been developed in the literature [8, 9, 40, 42, 67, 120, 125]. Generally these numerical methods can be classified into two main categories: interface-tracking methods and interface-capturing methods.

In the interface tracking methods, the moving interface is simulated by the sharp interface model. Numerically, it is explicitly represented by the computational mesh, and the mesh is updated when the interface evolves. The marker-particle methods [42, 125] were firstly presented for solving the sharp interface model of solid-state dewetting problems. This method is an explicit finite difference scheme, thus posing a very severe restriction on the numerical stability. Besides, at each time step, this algorithm requires re-meshing to redistribute the mesh points for the numerical stability. In consideration of these factors, the marker-particle method is tedious to perform and time-consuming, and the extension to the three dimensions is awkward. In [8], the authors recently have presented a parametric semi-implicit mixed finite element method for solving the sharp interface models, which they rigorously derived from the variation of the energy functionals. The numerical scheme they proposed is based on the automatically mesh-distributing scheme in [16], thus inheriting the good properties for mesh distribution. Their scheme can be applied to the case when the surface energy is weakly anisotropic and strongly anisotropic. Their ample numerical simulations and reports of some interesting theories on the two-dimensional solid-state dewetting demonstrate the parametric finite element method is powerful for the simulation of this problem.

The interface-capturing methods include the level set method and phase field method. They are based on an implicit representation of the surface by using the auxiliary function (level set function for level set method and phase function for phase field method) over a global domain, such that surface is implicitly captured via the zero contour of the auxiliary function. The interface-capturing methods to
compute the surface diffusion have been studied in the literature for level set methods \[31, 74, 107\] and phase field methods \[13–15, 25, 124\]. However, in the solid-state dewetting problem, in addition to the surface diffusion, the main difficulty for these interface-capturing methods lies in how to deal with the complex boundary conditions which result from the contact line migration. To our knowledge, the level set approach for solids-state dewetting problem is still a big challenge due to the complicated boundary conditions. On the other hand, Jiang et al. \[66\] first proposed a phase field model for simulating the solid-state dewetting with isotropic surface energy. The model includes the Cahn-Hilliard equation with degenerate mobility and nonlinear boundary conditions along the substrate. By making use of discrete cosine transforms (DCT) and discrete sine transforms (DST), they also proposed a highly efficient, stabilized, semi-implicit algorithm for solving the model. The numerical simulations obtained via this phase field approach showed qualitatively excellent agreement with physical experiments. The extended model for weakly anisotropic surface energy has been recently presented in \[46\] together with a matched asymptotic analysis for the sharp interface limit.

For comparisons between the interface-tracking and interface-capturing methods, each one has its own advantages and disadvantages. The interface-tracking methods via the sharp-interface model can always give the correct physics about surface diffusion together with contact line migration for the solid-state dewetting, and it is computationally efficient since it is one dimension less in space compared to the phase field model. But it is very tedious and troublesome to handle topological changes, e.g., pinch-off events. On the other hand, the interface-capturing methods via the phase field model can in general handle automatically topological changes and complicated geometries, but the sharp-interface limits of these phase field models are still unclear \[76\], and efficient and accurate simulations for surface diffusion and solid-state dewetting problems by using these models are still not well developed.
1.5 Scope of this thesis

Solid-state dewetting problems have been extensively studied with different models and numerical methods. However, there are still some limitations for these approaches. Firstly, the sharp interface model in two dimensions has been rigorously derived and an efficient parametric finite element method has been proposed to solve it. However, their models are not easy to be extended to the full three dimensions. Secondly, the extension of the parametric finite element method to three dimensions is not straightforward. This motives us to focus the following issues in this thesis,

- In chapter 2, we study the solid-state dewetting via thermodynamic variation in two dimensions as a start. The equilibrium shape and its linear stability has been well analysed. The sharp interface model with anisotropic surface energies is derived based on the thermodynamic variation via Cahn-Hoffman vector formulation. Efficient and stable numerical scheme is designed to solve the fourth-order geometric curve evolution equations.

- In chapter 3, based on the velocity speed method and shape derivatives, we derive the fully three-dimensional sharp interface model for solid-state dewetting with anisotropic surface energy and rigid flat substrate. The model includes the anisotropic surface diffusion flow and contact line migrations.

- In chapter 4, we present parametric finite element methods for solving the sharp the sharp interface model in both isotropic and anisotropic case. Extensive numerical results are presented to show the convergence of the numerical methods, the morphological characteristics for thin film during solid-state dewetting, and so on.

- In chapter 5, we extend our sharp interface model to the cases when the anisotropy is strong and and when the substrate is curved. Besides, the migration laws for the toroidal thin film on a flat substrate have been investigated and a reduced model will be obtained via Onsager’s principle for describing
1.5 Scope of this thesis

the migration.

The main works of this thesis are based on the papers [10, 11, 135, 136].
Chapter 2

Modeling and Simulation in Two Dimensions

The solid-state dewetting problems in two dimensions have been well studied recently [8, 9, 67, 120] via the sharp interface models. In these works, the authors presented the chemical potential in the form of a multiplication of the surface stiffness and the curve curvature, that is

\[ \mu = (\gamma(\theta) + \gamma''(\theta))\kappa \Omega_0, \]  

(2.0.1)

where \( \gamma(\theta) + \gamma''(\theta) \) is the surface stiffness, \( \kappa \) is the curvature, \( \Omega_0 \) is the atomic volume. Based on the expression, a generalized Winterbottom construction was proposed for the anisotropic particles on substrates via the variational approach, and conditions for the stable equilibrium were presented [9]. The theory was then numerically validated by solving these sharp interface models with the parametric finite element method [8]. Moreover, many physical phenomena of the solid-state dewetting have been investigated, such as the Rayleigh instability and power law retraction. However, the extensions of this mathematical representation for the chemical potential as well as the numerical methods to three dimensions are tedious although a similar representation is presented by Herring [60] for the three-dimensional Gibbs-Thompson...
2.1 Interfacial energy and thermodynamic variation

Equation in local coordinates

\[
\mu \equiv \left(\gamma + \frac{\partial^2 \gamma}{\partial n_x^2}\right)\kappa_x + \left(\gamma + \frac{\partial^2 \gamma}{\partial n_y^2}\right)\kappa_y \Omega_0,
\]

where \(\kappa_x, \kappa_y\) are the two principle curvatures, \(n_x, n_y\) are the two corresponding angles in the two principle directions.

Therefore in this chapter, based on the Cahn-Hoffman \(\xi\)-vector, we will present a new approach to studying the solid-state dewetting in two dimensions, and this approach is easily generalised to the three-dimensional case. In addition, we will consider the equilibrium problems via the variational approach and predicate the equilibrium shape as well as its stability conditions. Based on this variation we can derive the dynamic, sharp interface model via the form of the Cahn-Hoffman \(\xi\)-vector formulation. This model includes the surface diffusion flow and relaxed contact angle conditions for describing the motion of the interface curve and migrations of the contact points, respectively. Moreover, a variational formulation of the model is proposed, and then a new parametric finite element method is applied to solve it. The strongly anisotropic surface energy will also be considered via the Willmore energy regularization. Extensive numerical results will be shown afterwards.

2.1 Interfacial energy and thermodynamic variation

As illustrated in Figure. 2.1, an open curve \(\Gamma = X(x(s), y(s))\), parameterized by the arc length \(s\), which separates the vapor and the thin film, attaches on the flat substrate (x-axis) with two contact points \(x_c^l\) and \(x_c^r\). Here \(\mathbf{n}\) is the unit normal vector that points to the vapor and \(\mathbf{\tau}\) is the unit tangential vector in the clockwise direction. The total interfacial surface energy can be written as

\[
W = \int_{\Gamma_{FV}} \gamma_{FV} \, d\Gamma_{FV} + \int_{\Gamma_{FS}} \gamma_{FS} \, d\Gamma_{FS} + \int_{\Gamma_{VS}} \gamma_{VS} \, d\Gamma_{VS}.
\]

Here \(\Gamma_{FV}, \Gamma_{FS}\) and \(\Gamma_{VS}\) represent the film/vapor, film/substrate and vapor/substrate interface respectively, and \(\gamma_{FV}, \gamma_{FS}, \gamma_{VS}\) represent the corresponding surface energy.
2.1 Interfacial energy and thermodynamic variation

Figure 2.1: A schematic illustration of solid thin film on a rigid, flat substrate (x-axis) in two dimensions with two contact points $x_c^l$ and $x_c^r$.

densities (surface energy per unit length). As is typical in solid-state dewetting problems, we assume that $\gamma_{FS}, \gamma_{VS}$ are constants, while $\gamma_{FV} = \gamma(n) \in C^2(S^1)$ depends on the orientation of the film/vapor interface. By dropping a constant part of the total energy, the total surface energy can be simplified into

$$W = \int_{\Gamma} \gamma(n) \, ds - \sigma (x_c^r - x_c^l),$$

with $\sigma = (\gamma_{VS} - \gamma_{FS})$.

To perform the first variation of the interfacial energy, we first introduce an independent parameter $\rho \in I = [0, 1]$ to parameterize a family of curves $\{\Gamma^\varepsilon\}$, with $\varepsilon \in [0, \varepsilon_0]$ representing the perturbation magnitude, that is

$$X(\rho, \varepsilon) : [0, 1] \times [0, \varepsilon_0] \rightarrow \mathbb{R}^2.$$  

Here we denote $\Gamma^\varepsilon = X(\cdot, \varepsilon), \Gamma = \Gamma^0 = X(\cdot, 0)$. The parameterization of $\Gamma^\varepsilon$ is assumed to satisfy that $|\partial_\rho X(\rho, \varepsilon)| > 0, \forall \rho \in [0, 1]$. Define the the variation vector field

$$V(\rho, \varepsilon) = \frac{\partial X(\rho, \varepsilon)}{\partial \varepsilon},$$
as the corresponding infinitesimal deformation. Moreover, we assume for every \( \epsilon \), \( V \in C^k(I) \times C^k(I) \) with \( k \in \mathbb{N} \). For simplicity, in the following we will use \( V_0 \) to denote \( V(\rho, 0) \). Given a functional \( F(\Gamma) \), then we can define the first variation as a limit

\[
d F(\Gamma; V) = \lim_{\epsilon \to 0} \frac{F(\Gamma^\epsilon) - F(\Gamma)}{\epsilon}. \tag{2.1.5}
\]

In order to obtain the first variation of the total energy \( W \) defined in Eq. (2.1.2), we present a lemma at first.

**Lemma 2.1.1.** Suppose \( \Gamma = X(s) \in C^2([0, L]) \times C^2([0, L]) \) is an open curve where \( s(0 \leq s \leq L) \) is the arc length. If \( F(\Gamma) = \int_\Gamma \gamma(\mathbf{n}) \ ds \) and \( V(\rho, \epsilon) \) is a smooth variation vector field, then we have

\[
d F(\Gamma; V) = - \int_\Gamma (\partial_s \xi)^\perp \cdot \mathbf{n}(\mathbf{n} \cdot V_0) \ ds +\left[ \xi^\perp \cdot V_0 \right]_{s=0}^{s=L}, \tag{2.1.6}
\]

where \( \perp \) represents the clockwise rotation of a vector by 90 degrees, \( \xi \) is Cahn-Hoffman vector.

**Proof.** We first assume \( \hat{\gamma} \) is the homogenous extension of \( \gamma \) from \( S^1 \) to \( \mathbb{R}^2 \),

\[
\hat{\gamma}(p) = |p| \gamma(p / |p|), \quad \forall p \in \mathbb{R}^2 \setminus \{0\}. \tag{2.1.7}
\]

Define the perturbation in Eq. (2.1.3), then based on the parameterisation of \( \Gamma \), and noting that \( \partial_\rho s(\rho, \epsilon) = |\partial_\rho X(\rho, \epsilon)| \), we have

\[
F(\Gamma^\epsilon) = \int_0^1 \gamma(n^\epsilon)|\partial_\rho X(\rho, \epsilon)| \ dr. \tag{2.1.8}
\]

We note the following expressions hold:

\[
\tau^\epsilon = \frac{\partial X(\rho, \epsilon)}{\partial s(\rho, \epsilon)}, \quad n^\epsilon = -(\tau^\epsilon)^\perp = -\frac{[\partial_\rho X(\rho, \epsilon)]^\perp}{|\partial_\rho X(\rho, \epsilon)|},
\]

\[
\nabla \hat{\gamma}(p) \cdot p = \gamma(p), \quad V_0 = V(\rho, 0) = \partial_\rho X(\rho, \epsilon)_{|\epsilon=0}. \tag{2.1.9}
\]
2.1 Interfacial energy and thermodynamic variation

Under the perturbation defined in Eq. (2.1.3), let \( X = X(s) = X(\rho, 0) \), we can expand the following terms at \( \varepsilon = 0 \),

\[
|\partial_\rho X(\rho, \varepsilon)| = |\partial_\rho X| + \frac{\partial_\rho X \cdot \partial_\rho V_0}{|\partial_\rho X|} \varepsilon + O(\varepsilon^2), \tag{2.1.10a}
\]

\[
n^e = n + \left[ \frac{\partial_\rho X \cdot \partial_\rho V_0}{|\partial_\rho X|^3} (\partial_\rho X)^\perp - \frac{(\partial_\rho V_0)^\perp}{|\partial_\rho X|} \right] \varepsilon + O(\varepsilon^2), \tag{2.1.10b}
\]

\[
\gamma(n^e) = \gamma(n) + \nabla \hat{\gamma}(n) \left[ \frac{\partial_\rho X \cdot \partial_\rho V_0}{|\partial_\rho X|^3} (\partial_\rho X)^\perp - \frac{(\partial_\rho V_0)^\perp}{|\partial_\rho X|} \right] \varepsilon + O(\varepsilon^2). \tag{2.1.10c}
\]

The variation then can be written as

\[
dF(\Gamma; V) = \lim_{\varepsilon \to 0} \frac{F(\Gamma^\varepsilon) - F(\Gamma)}{\varepsilon} = \int_0^1 \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left[ \gamma(n^e) |\partial_\rho X(\rho, \varepsilon)| - \gamma(n) |\partial_\rho X(\rho, 0)| \right] d\rho. \tag{2.1.11}
\]

Substituting the expansions Eq. (2.1.10a) and Eq. (2.1.10c) into above equation gives us

\[
dF(\Gamma; V) = \int_0^1 \nabla \hat{\gamma}(n) \cdot \left[ \frac{\partial_\rho X \cdot \partial_\rho V_0}{|\partial_\rho X|^3} (\partial_\rho X)^\perp - \frac{(\partial_\rho V_0)^\perp}{|\partial_\rho X|} \right] |\partial_\rho X| d\rho \\
+ \int_0^1 \gamma(n) \frac{\partial_\rho X \cdot \partial_\rho V_0}{|\partial_\rho X|} d\rho \\
= -\int_0^1 \nabla \hat{\gamma}(n) \cdot (\partial_\rho V_0)^\perp d\rho = \int_0^1 \nabla \hat{\gamma}(n)^\perp \cdot \partial_\rho V_0 d\rho. \tag{2.1.12}
\]

Integrating by parts, and noting the definition of Cahn-Hoffman \( \xi \)-vector, we obtain

\[
dF(\Gamma; V) = -\int_0^1 (\partial_s \xi)^\perp \cdot V_0 d\rho + \left[ \xi^\perp \cdot V_0 \right]_{\rho=0}^{\rho=1} \\
= -\int_0^1 (\partial_s \xi)^\perp \cdot V_0 ds + \left[ \xi^\perp \cdot V_0 \right]_{s=0}^{s=L}. \tag{2.1.13}
\]

By the definition of \( \xi \), and noting that \( H_\gamma(n) \cdot n = 0 \) where \( H_\gamma \) is the hessian of \( \hat{\gamma} \), it is easy to show that \( \partial_s (\xi) \cdot n = 0 \). Thus the first variation of the total energy can be rewritten

\[
dW(\Gamma; V) = -\int_0^1 (\partial_s \xi)^\perp \cdot n \ (n \cdot V_0) ds + \left[ \xi^\perp \cdot V_0 \right]_{s=0}^{s=L}. \tag{2.1.14}
\]
2.2 Equilibrium and its stability condition

Lemma 2.1.1 gives the variation of the energy functional $F(\Gamma)$ under arbitrary perturbation. Here for the open curve that represents the film/vapor interface, we should assume that the two endpoints of the curve are always attached to the substrate. In other words, under this perturbation, the variation vector field should satisfy

$$V(0,0) \parallel x^+, \quad V(1,0) \parallel x^+, \quad (2.1.15)$$

where $x^+ = (1,0)$. Let $V_0 = (V_x, V_y)$, by lemma 2.1.1, we can directly obtain the first variation of the energy functional $W$ defined in Eq. (2.1.2),

$$dW(\Gamma; V) = -\int_\Gamma (\partial_s \xi^1) \cdot n \left( n \cdot V_0 \right) \, ds + \left[ (\xi_2 - \sigma) V_x \right]_{s=L} - \left[ (\xi_2 - \sigma) V_x \right]_{s=0}. \quad (2.1.16)$$

2.2 Equilibrium and its stability condition

Physical systems tend to move towards their equilibriums in the direction of decreasing the total energy. This principle can be mathematically formulated via the thermodynamic variation. The equilibrium shape equation can be obtained via the first variation of the energy functional. The second variation of the energy is often used to study the stability. So in this section, we will consider the equilibrium shape of solid-state dewetting via the thermodynamic variation approach.

2.2.1 Equilibrium shapes

The solid-state dewetting equilibrium problem can be written as a minimization of the total surface energy subject to the constraint of constant volume:

$$\min_{\Omega} W := \int_\Gamma \gamma(n) ds - \sigma(x^c_e - x^l_e) \quad s.t. \quad |\Omega| = \text{const.} \quad (2.2.1)$$

We first give a lemma about the first variation of area of the enclosed region $\Omega$.

**Lemma 2.2.1.** Suppose $\Gamma = X(s) = (x(s), y(s)) \in C^1([0,L]) \times C^1([0,L])$ is an open curve with two endpoints attached to the $x$–axis. Let $A$ denote the total area
2.2 Equilibrium and its stability condition

enclosed by $\Gamma$ and the $x$-axis, then we have

$$A(\Gamma) = \int_\Gamma y \partial_s x \, ds, \quad dA(\Gamma; V) = \int_\Gamma V_0 \cdot n \, ds.$$  \hfill (2.2.2)

Proof. The enclosed area can be obtained based on the divergence theorem

$$A(\Gamma) = \frac{1}{2} \int_\Gamma \mathbf{X} \cdot n \, ds.$$  \hfill (2.2.3)

The unit normal vector can be expressed as $n = (-\partial_s y, \partial_s x)$. Besides, noting that $y(0) = y(L) = 0$, then integrating by part, we can obtain

$$A(\Gamma) = \frac{1}{2} \int_\Gamma (y \partial_s x - x \partial_s y) \, ds$$

$$= \frac{1}{2} \int_\Gamma y \partial_s x \, ds + \frac{1}{2} \int_\Gamma \partial_s xy \, ds - (xy)_{s=L}^{s=0} = \int_\Gamma y \partial_s x \, ds.$$  \hfill (2.2.4)

Now based on the perturbation defined in Eq. (2.1.3) and the corresponding parametrization of $\Gamma^\epsilon$ on $[0,1]$, we have

$$dA(\Gamma; V) = \lim_{\epsilon \to 0} \frac{A(\Gamma^\epsilon) - A(\Gamma)}{\epsilon} = \int_0^1 \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left[ y(\rho, \epsilon) \partial_\rho x(\rho, \epsilon) - y(\rho, 0) \partial_\rho x(\rho, 0) \right] \, d\rho$$

$$= \int_0^1 V_y \partial_\rho x \, d\rho - \int_0^1 V_x \partial_\rho y \, d\rho + yV_x \bigg|_{\rho=0}^{\rho=1} = \int_\Gamma V_0 \cdot n \, ds.$$  \hfill (2.2.5)

This directly gives the first variation of enclosed area.

The equilibrium shape is obtained when the first variation of the total surface energy vanishes, thus we have the following lemma from [9]:

**Definition 2.2.1** (Equilibrium shapes [9]). If an open curve $\Gamma_e = (x(s), y(s)) \in C^2([0, L]) \times C^2([0, L])$, where $L$ is the arc length of $\Gamma_e$, satisfies $dW(\Gamma_e; V) \equiv 0$, where $V$ is a smooth vector field satisfying $\int_{\Gamma_e} n \cdot V_0 \, ds \equiv 0$, then it is the equilibrium shape of solid-state dewetting problem (2.2.1).

Based on the definition of equilibrium shape of solid state dewetting problem [9], we have

**Lemma 2.2.2.** Assume there is a curve satisfies $\Gamma_e = (x(s), y(s)) \in C^2[0, L]$, where $L$ is the arc length of $\Gamma_e$. Then if $\Gamma_e$ is an equilibrium shape of solid state dewetting...
2.2 Equilibrium and its stability condition

problem (2.2.1) if and only if the following two conditions are satisfied:

\[-\partial_s(\xi^\perp) \cdot n = C, \quad \forall s \in [0, L], \quad (2.2.6)\]
\[\xi_2 \bigg|_{s=0} - \sigma = 0, \quad \xi_2 \bigg|_{s=L} - \sigma = 0. \quad (2.2.7)\]

Here the constant \(C\) is determined by the total volume of the thin film.

**Proof.** The procedure of the proof for this lemma is similar to the proof in [9], so we omit it. \(\square\)

The above lemma is expressed in the form of the Cahn-Hoffman \(\xi\)-vector, which is the same as the lemma given in [9]. Eq. (2.2.6) could be written in a different expression

\[\nabla_s \cdot \xi = (\partial_s \xi) \cdot \tau = C, \quad \forall s \in [0, L], \quad (2.2.8)\]

which can be extended to the three-dimensional case directly, see Chapter 3. Eq. (2.2.7) can be regarded as the anisotropic Young equation. If the interfacial energy is isotropic, we obtain that \(\xi = n\), and on the boundary (two contact points), Eq. (2.2.7) collapses to \(\cos \theta_c = \sigma\) with \(\theta_c\) denoting the contact angle.

2.2.2 Stability condition

In absence of the substrate, the equilibrium shape that minimise the energy functional \(\int_{\Gamma} \gamma(n) \, ds\) while preserving the total volume is given by Wulff shape [126]. When \(\gamma(n) = 1\), this problem reduces to the well-known isopermetric problem. The stability of the corresponding equilibrium shape: sphere has been proved [12, 121] based on the second variational approach. The stability of Wulff shape for general anisotropy has been widely studied [87, 122]. The result can be concluded as: if the anisotropy satisfies the convexity assumption, that is

\[H_q(p)q \cdot q \geq \lambda_0 |q|, \quad \forall q \in S^1, p \cdot q = 0, \quad (2.2.9)\]

where \(\lambda_0\) is a positive constant, then only closed, orientated, stable critical points of the energy functional is Wulff shape, up to scaling and translation. However,
when the convexity condition is not satisfied, we knew that ears appear in the Wulff envelope ($\xi$-plot) as some orientations are missing on the Wulff shape. The Wulff envelope truncated by a flat substrate line could produce multiple equilibrium shapes [67]. On the other hand, the condition for the stable equilibrium is that its second variation of the energy functional is non-negative for all variations that preserving the area. So in this section, we perform the second variation of the energy functional and derive the stability conditions of the equilibrium shape for solid-state dewetting. For simplicity, and avoiding using the Jacobia operator for a vector variation field, we assume the perturbation is expressed in one parameter, that is

$$X(\rho, \varepsilon) = X(\rho, 0) + \varepsilon X^1(\rho).$$ (2.2.10)

Thus we have $V_0 = X^1(\rho)$, and we can define the second variation

$$d^2F(\Gamma; V) = d^2F(\Gamma^\varepsilon)|_{\varepsilon=0}.$$ (2.2.11)

We have the following lemma for the second variation.

**Lemma 2.2.3.** Suppose $\Gamma = X(s) \in C^2([0, L]) \times C^2([0, L])$ is an open curve where $s(0 \leq s \leq L)$ is the arc length and assume the perturbation is given by (2.2.10). Let $F(\Gamma) = \int_{\Gamma} \gamma(n)|\partial_\rho X(\rho, \varepsilon)| d\rho$. Then we have

$$d^2F(\Gamma; V) = \int_{\Gamma} H_{\gamma}(n)\tau \cdot \tau(\partial_\rho V_0 \cdot n)^2 ds,$$ (2.2.12)

where $\tau$ is the unit tangential vector.

**Proof.** Here we can write the second variation as

$$d^2F(\Gamma; V) = \frac{d^2}{d\varepsilon^2} \int_0^1 \gamma(n^\varepsilon)|\partial_\rho X(\rho, \varepsilon)| d\rho.$$ (2.2.13)

Expand $\Gamma(n^\varepsilon)$ and $|\partial_\rho X(\rho, \varepsilon)|$ up to second order under the perturbation defined in
Eq. (2.2.10), we obtain (see Appendix. A for detailed derivation),

\[
\frac{\partial X(\rho, \varepsilon)}{\partial \rho X} = 1 + (\tau \cdot \partial_s V_0)\varepsilon + \frac{1}{2} (\partial_s V_0 \cdot \partial_s V_0 - (\tau \cdot \partial_s V_0)^2)\varepsilon^2 + O(\varepsilon^3), \quad (2.2.14a)
\]

\[
\gamma(n^*) = \gamma(n) + \left[ -\gamma(n)(\tau \cdot \partial_s V_0) - \nabla \hat{\gamma}(n) \cdot (\partial_s V_0)^\perp \right] \varepsilon
+ \frac{1}{2} \left[ 2\nabla \hat{\gamma}(n) \cdot (\partial_s V_0 \cdot \tau)(\partial_s V_0)^\perp - \gamma(n)(\partial_s V_0 \cdot \partial_s V_0)
+ 3\gamma(n)(\tau \cdot \partial_s V_0)^2 + H_\gamma(n)(\partial_s V_0)^\perp \cdot (\partial_s V_0)^\perp \right] \varepsilon^2 + O(\varepsilon^3). \quad (2.2.14b)
\]

Extracting all \(O(\varepsilon)\) terms of \(\gamma(n^*)|\partial_\rho X(\rho, \varepsilon)|\), we get

\[
\frac{d^2}{d\varepsilon^2} \left( \gamma(n^*)|\partial_\rho X(\rho, \varepsilon)| \right) |_{\varepsilon=0} = -2|\partial_\rho X| \left[ \gamma(n)(\tau \cdot \partial_s V_0) + \nabla \hat{\gamma}(n) \cdot (\partial_s V_0)^\perp \right] (\tau \cdot \partial_s V_0)
+ |\partial_\rho X| \gamma(n) \left[ \partial_s V_0 \cdot \partial_\rho V_0 - (\tau \cdot \partial_s V_0)^2 \right]
+ |\partial_\rho X| \left[ 2\nabla \hat{\gamma}(n) \cdot (\partial_s V_0 \cdot \tau)(\partial_s V_0)^\perp - \gamma(n)(\partial_s V_0 \cdot \partial_s V_0)
+ 3\gamma(n)(\tau \cdot \partial_s V_0)^2 + H_\gamma(n)(\partial_s V_0)^\perp \cdot (\partial_s V_0)^\perp \right]
= H_\gamma(n)(\partial_s V_0)^\perp \cdot (\partial_s V_0)^\perp |\partial_\rho X|. \quad (2.2.15)
\]

The last equality of above equations is due to a simple reduction. Thus we can directly obtain that

\[
d^2 F(\Gamma; V) = \int_0^1 H_\gamma(n)(\partial_s V_0)^\perp \cdot (\partial_s V_0)^\perp |\partial_\rho X| \, d\rho
= \int_\Gamma H_\gamma(n)(\partial_s V_0)^\perp \cdot (\partial_s V_0)^\perp \, ds. \quad (2.2.16)
\]

Express \((\partial_s V_0)^\perp\) into the linear combination of normal and tangential parts

\[
(\partial_s V_0)^\perp = [((\partial_s V_0)^\perp \cdot n]n + [((\partial_s V_0)^\perp \cdot \tau] \tau
= [\partial_s V_0 \cdot \tau] \tau - [\partial_s V_0 \cdot n] \tau. \quad (2.2.17)
\]

Note that \(H_\gamma(n)n = 0\), we obtain

\[
d^2 F(\Gamma; V) = \int_\Gamma H_\gamma(n) \tau \cdot (\partial_s V_0 \cdot n) \, ds. \quad (2.2.18)
\]
According to lemma 2.2.3, we know that the second variation under the perturbation Eq. (2.2.10) is given directly as

\[ d^2W(\Gamma; V) = \int_\Gamma H_\gamma(n)\tau \cdot \tau(\partial_s V_0 \cdot n)^2 \, ds. \]  \hspace{1cm} \text{(2.2.19)}

Thus the stability condition for an equilibrium shape is given by

\[ H_\gamma(n)\tau \cdot \tau > 0. \]  \hspace{1cm} \text{(2.2.20)}

The same stability condition for an equilibrium shape has been derived in [9] with the surface stiffness \( \gamma(\theta) + \gamma''(\theta) > 0 \). Here the condition is presented in a different form. These two forms are equivalent. Based on this stability condition, the author proposed a generalized Winterbottom construction to include all the possible multiple equilibrium shapes for strongly anisotropic case.

2.3 The sharp interface model

In this section, based on thermodynamic variation, the sharp interface model will be developed. The mass conservation and energy dissipation for the dynamic model will be shown afterwards.

In view of Eq. (2.1.14), the first variation of the total energy with respect to the moving interface and two contact points give us:

\[ \frac{\delta W}{\delta \Gamma} = -[\partial_s \xi^\perp] \cdot n, \]  \hspace{1cm} \text{(2.3.1a)}

\[ \frac{\delta W}{\delta x_c^l} = -(\xi_2|_{s=0} - \sigma), \]  \hspace{1cm} \text{(2.3.1b)}

\[ \frac{\delta W}{\delta x_c^r} = (\xi_2|_{s=L} - \sigma). \]  \hspace{1cm} \text{(2.3.1c)}

From the anisotropic Gibbs-Thomson relation [113], the chemical potential is defined as

\[ \mu = \Omega_0 \frac{\delta W}{\delta \Gamma}, \]  \hspace{1cm} \text{(2.3.2)}
with \( \Omega_0 \) representing the atomic volume. The normal velocity \( v_n \) of the curve \( \Gamma \) is given by surface diffusion flow

\[
v_n = \frac{D_s \nu \Omega_0}{k_B T} \partial_{ss} \mu. \tag{2.3.3}
\]

In these expressions, \( D_s \) is the surface diffusivity, \( k_B T \) is the thermal energy, \( \nu \) is the number of diffusing atoms per unit length.

The motions of the two contact points are determined by the time-dependent Ginzburg-Landau kinetic equations

\[
\frac{dx_l(t)}{dt} = -\frac{\delta W}{\delta x_l}, \quad \frac{dx_r(t)}{dt} = -\frac{\delta W}{\delta x_r}, \tag{2.3.4}
\]

with \( \eta \) denoting the contact point mobility.

### 2.3.1 The dimensionless equations

Now take the characteristic length scale and characteristic surface energy scale as \( L \) and \( \gamma_0 \) respectively, by choosing the time scale as \( \frac{L^4}{B \gamma_0} \) with \( B = \frac{D_s \nu \Omega_0^2}{k_B T} \), and the contact line mobility is scaled by \( \frac{B}{T} \). Then the dimensionless sharp interface model for solid-state dewetting can be written as,

\[
\partial_t X = \partial_{ss} \mu \mathbf{n}, \quad 0 < s < L(t), \quad t > 0, \tag{2.3.5}
\]

\[
\mu = -[\partial_s \xi]^\perp \cdot \mathbf{n}, \quad \xi = \nabla \gamma(n). \tag{2.3.6}
\]

where \( X(x(s,t), y(s,t)) \) denotes the moving interface, \( L := L(t) \) represents the total length of the moving interface at time \( t \), \( \xi = (\xi_1, \xi_2) \), together with the following boundary conditions:

(i) contact point condition

\[
y(0, t) = 0, \quad y(L, t) = 0, \quad t \geq 0, \tag{2.3.7}
\]

(ii) relaxed contact angle condition

\[
\frac{dx_l}{dt} = \eta(\xi_2 - \sigma)|_{s=0}, \quad \frac{dx_r}{dt} = -\eta(\xi_2 - \sigma)|_{s=L}, \quad t \geq 0, \tag{2.3.8}
\]
(iii) zero-mass flux condition

\[ \partial_s \mu(0, t) = 0, \quad \partial_s \mu(L, t) = 0, \quad t \geq 0, \]  

(2.3.9)

\(0 < \eta < \infty\) denotes the contact line mobility, \(\sigma = \frac{\gamma \nu_s - \gamma \nu_g}{\eta_0}\).

### 2.3.2 Mass conservation and energy dissipation

In this section, we show that the mass is conserved and total energy is decreasing under the dynamics of the above sharp-interface model.

**Proposition 2.3.1** (Mass conservation and energy dissipation). Let \(\Gamma(t) = X(s, t)\) be the exact solution of Eqs. (2.3.5), (2.3.6) coupled with the boundary conditions (2.3.7)-(2.3.9), and the initial curve is given by \(\Gamma(0) = (x_0(s), y_0(s))\). Then the total mass of the thin film is conserved during the evolution, i.e.,

\[ A(t) \equiv A(0) = \int_{\Gamma(0)} y_0(s) \partial_s x_0(s) \, ds, \quad t \geq 0. \]  

(2.3.10)

and the total energy of the thin film is decreasing during the evolution, i.e.,

\[ W(t) \leq W(t_1) \leq W(0) = \int_{\Gamma(0)} \gamma(n) \, ds - (x_r(0) - x_l(0))\sigma, \quad t \geq t_1 \geq 0. \]  

(2.3.11)

**Proof.** From Eq. (2.2.2), by directly calculating the time derivative of \(A(t)\) and using lemma 2.2.1, we can obtain the following expression

\[ \frac{d}{dt} A(t) = \int_{\Gamma(t)} X_t \cdot n \, ds = \int_{\Gamma(t)} \mu_{ss} \, ds = 0. \]  

(2.3.12)

The last equality follows from the zero-mass flux boundary condition, and it indicates that the mass is conserved.

To obtain the time derivative of \(W(t)\), we can make use of the Eq. (2.1.16), but replace the perturbation parameter by the time \(t\), then we get:

\[ \frac{d}{dt} W(t) = -\int_{\Gamma} (\partial_s \xi)_{s=L(t)} \cdot X_t \, ds + (\xi_r|_{s=L(t)} - \sigma) \frac{dx_r}{dt} - (\xi_l|_{s=0} - \sigma) \frac{dx_l}{dt}. \]  

(2.3.13)
Now use (2.3.5) and (2.3.6) and the contact line moving boundary conditions (2.3.8), also note that \( \partial_s \xi \cdot n = 0 \), we have

\[
\frac{d}{dt} W(t) = \int_{\Gamma(t)} \mu \partial_{ss} \mu \, ds - \frac{1}{\eta} \left[ \left( \frac{dx_c^l}{dt} \right)^2 + \left( \frac{dx_c^r}{dt} \right)^2 \right] \\
= - \int_{\Gamma(t)} (\partial_s \mu)^2 \, ds - \frac{1}{\eta} \left[ \left( \frac{dx_c^l}{dt} \right)^2 + \left( \frac{dx_c^r}{dt} \right)^2 \right] \leq 0. \tag{2.3.14}
\]

The last inequality immediately implies the energy dissipation.

\section*{2.4 A parametric finite element method (PFEM)}

In this section, we propose a parametric finite element method for solving the sharp interface model. The governing equations for the model belong to fourth order geometric curve evolution equations coupled with dynamic boundary conditions.

\subsection*{2.4.1 Variational formulation}

In order to present the variational formulation of the problem (2.3.5)-(2.3.9), we introduce a new time-independent spatial variable \( \rho \in I := [0, 1] \) and use it to parameterize the curve \( \Gamma(t) \) instead of using the arc length \( s \). More precisely, if we assume that \( \Gamma(t) \) is a family of open curves in the plane, where \( t \in [0, T] \) with \( T > 0 \) a fixed time, then we can parameterize the curves as

\[
\Gamma(t) = X(\rho, t) : I \times [0, T] \to \mathbb{R}^2. \tag{2.4.1}
\]

It should be noted that the relationship between the variable \( \rho \) and the arc length \( s \) can be given by \( s(\rho, t) = \int_0^\rho |\partial_q X| \, dq \), which immediately implies that \( \partial_\rho s = |\partial_\rho X| \).

Introduce the functional space with respect to the evolution curve \( \Gamma(t) \) as

\[
L^2(I) = \{ u : I \to \mathbb{R}, \text{ and } \int \int |u(s)|^2 ds < +\infty \}, \tag{2.4.2}
\]

equipped with the \( L^2 \) inner product

\[
\langle u, v \rangle_\Gamma := \int_{\Gamma(t)} u(s)v(s) \, ds = \int_I |u(s(\rho, t))v(s(\rho, t))| \partial_\rho X \, d\rho, \quad \forall u, v \in L^2(I). \tag{2.4.3}
\]
for any scalar (or vector) functions. Note that the defined space $L^2(I)$ can be viewed as the conventional $L^2$ space but equipped with different weighted inner product associated with the moving curve $\Gamma(t)$. Define the functional space for the solution of the solid-state dewetting problem as

$$H^1_{a,b}(I) = \{ u \in H^1(I) : u(0) = a, u(1) = b \},$$

(2.4.4)

where $a$ and $b$ are two given constants which are related to the two moving contact points at time $t$, respectively, and $H^1(I) = \{ u \in L^2(I) : \partial_s u \in L^2(I) \}$ is the standard Sobolev space with the derivative taken in the distributional or weak sense. For the simplicity of notations, we denote the functional space $H^1_0(I) := H^1_0,0(I)$. By using the integration by parts, we can obtain the variational problem for the solid-state dewetting problem with isotropic/weakly anisotropic surface energy: given an initial curve $\Gamma(0) = X(\rho, 0) = X_0(s)$ with $s = L_0 \rho$ for $\rho \in I$, for any time $t \in (0, T]$, find the evolution curves $\Gamma(t) = X(\rho, t) \in H^1_{a,b}(I) \times H^1_0(I)$ with the $x$-coordinate positions of moving contact points $a = x^l_c(t) \leq x^r_c(t) = b$, the chemical potential $\mu(\rho, t) \in H^1(I)$ such that

$$\frac{d}{dt} \langle n, \varphi \rangle_\Gamma + \langle \partial_s \mu, \partial_s \varphi \rangle_\Gamma = 0, \quad \forall \varphi \in H^1(I),$$

(2.4.5)

$$\langle \mu n, \omega \rangle_\Gamma - \langle \xi^\perp, \partial_s \omega \rangle_\Gamma = 0, \quad \forall \omega \in H^1_0(I) \times H^1_0(I),$$

(2.4.6)

coupled with that the positions of the moving contact points, i.e., $x^l_c(t)$ and $x^r_c(t)$, which are updated by the boundary condition Eq. (2.3.8). Here the $L^2$ inner product $\langle \cdot, \cdot \rangle_\Gamma$ and the differential operator $\partial_s$ depend on the curve $\Gamma := \Gamma(t)$. In fact, Eq. (2.4.5) is obtained by re-formulating (2.3.5) as $n \cdot \partial_t X = \partial_s \mu$, multiplying the test function $\varphi$, integrating over $\Gamma$, integration by parts and noticing the boundary condition (2.3.9). Similarly, Eq. (2.4.6) is derived by re-formulating (2.3.6) as $\mu n = -\partial_s (\xi^\perp)$, multiplying the vector valued test function $\omega$, and Eq. (2.4.6) is obtained. Here we develop the variational formulation in the form of Cahn-Hoffman $\xi$-vector. A similar variational formulation was proposed by J.W. Barrett [19, 24] for discretizing the corresponding variational problem with applications to thermal grooving and sintering in materials science. An advantage of their method is that
2.4 A parametric finite element method (PFEM)

they can prove a stability bound for a special class of anisotropic surface energy density. For our variational formulation (2.4.5)-(2.4.6), the discretization could be applied to more general anisotropies. Another variational formulation proposed in [8], based on $\mu = (\gamma + \gamma'')\kappa$, includes one more equations for the curvature. This makes the variational formulation more complicated and stability bounds for that discrete scheme are not available.

In the following, we show that the weak solution to the variational formulation (2.4.5) and (2.4.6) also satisfies the two propositions, i.e. mass conservation and energy dissipation during the evolution.

**Proposition 2.4.1** (Mass conservation and energy dissipation for weak solution).

Assume $(X(\rho,t), \mu(\rho,t))$ be the weak solution of the weak formulation (2.4.5) and (2.4.6), the initial curve is given as $\Gamma(0) = (x_0(s), y_0(s))$, then the total mass of the thin film is conserved during the evolution, i.e.,

$$A(t) \equiv A(0) = \int_{\Gamma(0)} y_0(s) \partial_s x_0(s) \, ds, \quad t \geq 0. \quad (2.4.7)$$

Furthermore, if we assume that $X(\rho,t) \in C^1(C^2(I); [0, T]) \times C^1(C^2(I); [0, T])$, then the total energy of the thin film is decreasing during the evolution, i.e.,

$$W(t) \leq W(t_1) \leq W(0) = \int_{\Gamma(0)} \gamma(n) \, ds - (x^r_c(0) - x^l_c(0)) \sigma, \quad t \geq t_1 \geq 0. \quad (2.4.8)$$

**Proof.** From (2.2.2), similar to the proof of Proposition 2.3.1, by calculating the time derivative of $A(t)$ we can obtain the following expression

$$\frac{d}{dt} A(t) = \int_{\Gamma(t)} X_t \cdot n \, ds. \quad (2.4.9)$$

By choosing the test function in Eq. (2.4.5) as $\varphi = 1$, we can obtain that:

$$\frac{d}{dt} A(t) = \int_{\Gamma(t)} X_t \cdot n \, ds = - \int_{\Gamma(t)} \mu_s \varphi_s \, ds = 0.$$

Hence, the weak solution to the variational formulation satisfies the mass conservation during the evolution.
Similarly, from Eq. (2.1.12), we can also get the following equation for the time derivative of the energy:

$$\frac{d}{dt} W(t) = \int_{\Gamma(t)} \xi^\perp \cdot \partial_s (\partial_t X) \, ds - \sigma \left( \frac{dx_c^r}{dt} - \frac{dx_c^l}{dt} \right). \quad (2.4.10)$$

Now we can choose the test function in Eqs. (2.4.5) and (2.4.6) as

$$\varphi = \mu, \quad \omega = \partial_t X - \frac{dx_c^l}{dt} \zeta_1 - \frac{dx_c^r}{dt} \zeta_2, \quad (2.4.11)$$

where \( \zeta_1 = (\zeta_1(\rho), 0) \) and \( \zeta_2 = (\zeta_2(\rho), 0) \) with \( \zeta_1 \in H^1_{0,0}(I) \) and \( \zeta_2 \in H^1_{0,1}(I) \) such that \( \omega \in H^1_0(I) \times H^1_0(I) \), then we can simplify the equation (2.4.10) as

$$\frac{d}{dt} W(t) = - \frac{1}{\eta} \left[ \left( \frac{dx_c^l}{dt} \right)^2 + \left( \frac{dx_c^r}{dt} \right)^2 \right] - \int_{\Gamma(t)} \left( \partial_s \mu \right)^2 \, ds - \int_{\Gamma(t)} \frac{dx_c^l}{dt} \int \zeta_1 \cdot (\mu n + \partial_s \xi^\perp) \, ds - \int_{\Gamma(t)} \frac{dx_c^r}{dt} \int \zeta_2 \cdot (\mu n + \partial_s \xi^\perp) \, ds \leq - \int_{\Gamma(t)} \frac{dx_c^l}{dt} \int \zeta_1 \cdot (\mu n + \partial_s \xi^\perp) \, ds - \int_{\Gamma(t)} \frac{dx_c^r}{dt} \int \zeta_2 \cdot (\mu n + \partial_s \xi^\perp) \, ds.$$

The assumption \( X(\rho, t) \in C^1(C^2(I); [0, T]) \times C^1(C^2(I); [0, T]) \) implies that \( \mu n + \partial_s \xi^\perp \in L^2(I) \times L^2(I) \), and taking \( \| \zeta_1 \|_{L^2} \) and \( \| \zeta_2 \|_{L^2} \) as small as possible, we obtain

$$\frac{d}{dt} W(t) \leq 0, \quad (2.4.12)$$

which immediately implies the energy dissipation.

2.4.2 Semi-discretization

Before we go to the full-discrete mixed form finite element scheme for the variational formulation Eq. (2.4.5) and (2.4.6), we first consider the semi-discrete scheme, in which we only divide the space (the domain \( I \)). A uniform partition of \( I \) is given as: \( \rho \in I = [0, 1] = \bigcup_{j=1}^N I_j = \bigcup_{j=1}^N [\rho_{j-1}, \rho_j] \), where \( N \) denotes the number of divided small intervals, and \( \rho_j = jh \) denotes the interval nodes with the uniform interval length \( h = 1/N \).

Let \( \Gamma(t) = X^h(\cdot, t) \) be the numerical approximation to the moving curve \( \Gamma = X(\cdot, t) \) at the time \( t \). Define the finite element spaces to approximate \( H^1(I) \) and
H^1_{a,b}(I)$ with $a$ and $b$ two given constants as
\begin{align}
V^h := \{ u \in C(I) : u \mid_{I_j} \in P_1, \quad \forall j = 1, 2, \ldots, N \} \subseteq H^1(I), \\
V^h_{a,b} := \{ u \in V^h : u(0) = a, \ u(1) = b \} \subseteq H^1_{a,b}(I),
\end{align}
where $P_1$ denotes the polynomial with degrees at most 1. For simplicity, we denote $V^h_0 = V^h_{0,0}$. Since we use the $P_1$ (linear) elements to approximate the moving curves, therefore the numerical solutions for moving interfaces are polygonal curves, set $h(t) = X^h(\rho_j, t) - X^h(\rho_{j-1}, t)$, where $j = 1 \rightarrow N$, we have: $X^h(\rho, t) = \bigcup_{j=1}^{N} h_j(t)$, and the tangential and normal vector of the numerical solution $\Gamma$ are step functions with possible discontinuities or jumps at nodes $\rho_j$, the unit tangential vector can be computed as $\tau^h_j = \tau^h \mid_{I_j} = \frac{h_j}{\|h_j\|}$ and the normal vector can be numerically computed as $n^h = -[\tau^h]_\bot$.

Furthermore, if $u$ and $v$ are two piecewise continuous scalar or vector functions defined on the domain $I$, with possible jumps at the nodes $\{\rho_j\}_{j=1}^N$, we can define the mass lumped inner product $\langle \cdot, \cdot \rangle^h_\Gamma$ as
\begin{equation}
\langle u, v \rangle^h_\Gamma = \frac{1}{2} \sum_{j=1}^{N} |h_j| \bigg[ \big((u \cdot v)(\rho^{-}_j) + (u \cdot v)(\rho^{+}_{j-1})\big) \bigg],
\end{equation}
where $u(q^{-}_j)$ and $u(q^{+}_{j})$ represent the limit values at the the possible jump node $q_j$ from the left-hand side and the right-hand side, respectively.

Take $\Gamma^0 = X^0 \in V^h_{x_0(0),x_0(L_0)} \times V^h_0$ such that $X^0(\rho_j) = X_0(s^0_j)$ with $s^0_j = jL_0/ N = L_0 \rho_j$ for $j = 0, 1, \ldots, N$, now the semi-discrete scheme for the variation formulation (2.4.5) and (2.4.6) can be stated as following: given the initial curve $\Gamma(0) = X^h(\cdot, 0)$, for every time $t \in (0, T]$, find the evolution curves $\Gamma(t) = X^h(\cdot, t) \in V^h_{a,b} \times V^h_0$ with the $x$-coordinate positions of moving contact points $a = x^c(t) \leq x^c(t) = b$, the chemical potential $\mu^h(\cdot, t) \in V^h$ such that
\begin{align}
\langle \partial_t X^h, \varphi^h \rangle^h_\Gamma + \langle \partial_s \mu^h, \partial_s \varphi^h \rangle^h_\Gamma = 0 \quad \forall \varphi^h \in V^h, \\
\langle \mu^h n^h, \omega^h \rangle^h_\Gamma - \langle \xi^h n^h, \partial_t \omega^h \rangle^h_\Gamma = 0 \quad \forall \omega^h \in V^h_0 \times V^h_0,
\end{align}
where $x^c_l(t)$ and $x^c_r(t)$ are determined by (2.3.8).
Proposition 2.4.2 (Mass conservation and energy dissipation for semi-discrete solutions). Assume \( X^h(t) \in \mathcal{V}_{a,b}^h \times \mathcal{V}_0^h \) and \( \mu^h \in \mathcal{V}^h \) are the discrete solutions of the Eqs (2.4.16) and (2.4.17). Given \( \Gamma^h(0) = X^0(\rho) = \bigcup_{j=1}^N h_j(0) \), then the mass of the thin film for the polygonal curves is conserved during the evolution, i.e.

\[
A^h(t) = A^h(0) = \frac{1}{2} \sum_{j=1}^N [x_0(\rho_j) - x_0(\rho_{j-1})] [y_0(\rho_j) + y_0(\rho_{j-1})], \quad t \geq 0. \tag{2.4.18}
\]

The total energy of the thin film for the polygonal curves is decreasing during the evolution if the mesh size \( h \) is small enough, i.e.

\[
W^h(t) \leq W^h(t_1) \leq W^h(0) = \sum_{j=1}^N \gamma(n_j^h(0)) h_j(0) - \sigma(x_c^h(0) - x_c^h(0)), \quad t \geq t_1 \geq 0, \tag{2.4.19}
\]

where \( n_j^h(0) = -\frac{h_j(0)}{h_h(0)} \), \( h_j(0) = X^0(\rho_j) - X^0(\rho_{j-1}) \), for \( 1 \leq j \leq N \), \( x_c^h(0) = x_0(1) \), \( x_c^h(0) = x_0(0) \).

Proof. Let \( X^h(\rho_j, t) = X_j^h(t) = (x_j, y_j) \), and note that \( y_0 = y_N = 0 \). Then the total mass of the thin film can be described as

\[
A^h(t) = \frac{1}{2} \sum_{j=1}^N (x_j - x_{j-1})(y_j + y_{j-1})
= \frac{1}{2} \sum_{j=1}^N x_j y_j - \frac{1}{2} \sum_{i=1}^N x_{j-1} y_{j-1} + \frac{1}{2} \sum_{i=1}^N (x_j y_{j-1} - x_{j-1} y_j)
= \frac{1}{2} \sum_{j=1}^N X^h_j \cdot (X^h_{j-1})^\perp. \tag{2.4.20}
\]

Then calculate the time derivative directly, we have:

\[
\frac{d}{dt} A^h(t) = \frac{1}{2} \sum_{j=1}^N \left[ \frac{d}{dt} X^h_j \cdot (X^h_{j-1})^\perp + X^h_j \cdot \frac{d}{dt} (X^h_{j-1})^\perp \right]
= \frac{1}{2} \sum_{j=1}^N \left[ \frac{d}{dt} X^h_j \cdot (X^h_{j-1})^\perp - \frac{d}{dt} X^h_{j-1} \cdot (X^h_j)^\perp \right]
= \frac{1}{2} \sum_{j=1}^N \left[ \frac{d}{dt} X^h_j + \frac{d}{dt} X^h_{j-1} \right] [X^h_{j-1} - X^h_j]^\perp
= \frac{1}{2} \sum_{j=1}^N \left| h_j \right| \left( \frac{d}{dt} X^h_j + \frac{d}{dt} X^h_{j-1} \right) \cdot n^h_j = \langle \partial_t X^h, n^h \rangle. \tag{2.4.21}
\]

If we choose \( \varphi_h = 1 \) in (2.4.16), we obtain

\[
\frac{d}{dt} A^h(t) = -\langle \partial_t \mu^h, \partial_t 1 \rangle^h = 0. \tag{2.4.22}
\]
Thus, from equation (2.4.22), the area enclosed by the interface and substrates is conserved.

For the total energy, note that the total energy of the the thin film can be described as

$$W_h(t) = \sum_{i=1}^{N} \hat{\gamma}(-[h_j]^{\perp}) - \sigma(x_c^e - x_c^l), \tag{2.4.23}$$

By calculating the time derivative directly, we can obtain:

$$\frac{d}{dt}W_h(t) = \sum_{j=1}^{N} \nabla\hat{\gamma}(-[h_j]^{\perp}) \frac{d}{dt}(-[e_j]^{h\perp}) - \sigma(\frac{dx_r}{dt} - \frac{dx_l}{dt})$$

$$= \sum_{j=1}^{N} |\xi_j^{h\perp}| \frac{d}{dt} h_j - \sigma(\frac{dx_r}{dt} - \frac{dx_l}{dt}). \tag{2.4.24}$$

Note that $h_j = \partial_{\rho}X^h(t)\mid_{I_j}$, then

$$\frac{d}{dt}W_h(t) = \left(\left[\xi^{h\perp}, \partial_{\rho}(\partial_{\rho}X^h)\right]_{\Gamma} - \sigma(\frac{dx_r}{dt} - \frac{dx_l}{dt})\right). \tag{2.4.25}$$

Now we pick the following test functions for the semi-discrete scheme (2.4.16) and (2.4.17),

$$\varphi_h = \mu^h, \quad \omega_h = \partial_t X^h - \frac{dx_r}{dt} \zeta_1 - \frac{dx_l}{dt} \zeta_2, \tag{2.4.26}$$

where $\zeta_1 = (\zeta_1, 0), \zeta_2 = (\zeta_2, 0)$ and $\zeta_1, \zeta_2$ are the $P^1$ nodial basic function at point $q_0$ and $q_N$ respectively. The choice of $\zeta_1$ and $\zeta_1$ can ensure the $\omega \in V_0^h \times V_0^h$, then we have:

$$\frac{d}{dt}W_h(t) = \langle [\xi^{h\perp}, \partial_{\rho}(\partial_{\rho}X^h)]_{\Gamma} - \sigma(\frac{dx_r}{dt} - \frac{dx_l}{dt})\rangle$$

The first term and last term are always smaller that 0. For the second and third term, they can be bounded by $Ch(|\frac{dx_r}{dt}| + |\frac{dx_l}{dt}|)$, thus if $h$ is small enough, we can
ensure
\[
\frac{d}{dt} W^h(t) \leq 0, \quad (2.4.27)
\]
which immediately implies the energy dissipation.

### 2.4.3 Full-discretization

In this section, we will introduce the full-discrete finite element method for the variational formulation (2.4.5) and (2.4.6). We subdivide the time interval as \(0 = t_0 < t_1 < \ldots < t_{M-1} < t_M = T\) with \(\tau_m = t_{m+1} - t_m\). Let \(\Gamma^m := X^m, n^m\) and \(\mu^m\) be the numerical approximations of the moving curve \(\Gamma(t_m) := X(\cdot, t_m)\), the normal vector \(n\) and the chemical potential \(\mu\) at time \(t_m\), respectively. For simplicity, we denote \(X^m(\rho_j) = (x^m_j, y^m_j)\). Take \(\Gamma^0 = X^0(0) \in V^h_0 \times V^h_0\) such that \(X^0(\rho_j) = X^0(\tau^0_j)\) with \(\rho_j = 0, 1, \ldots, N\), then a semi-implicit parametric finite element method (PFEM) for the variational problem (2.4.5)-(2.4.6) can be given as: for \(m \geq 0\), find \(\Gamma^{m+1} = X^{m+1} \in V^h_{a,b} \times V^h_0\) with the \(x\)-coordinate positions of the moving contact points \(a := x^c_1(t_{m+1}) \leq b := x^c_2(t_{m+1})\) and \(\mu^{m+1} \in V^h\) such that

\[
\begin{align*}
\left(\frac{X^{m+1} - X^m}{\tau_m}, \varphi_h n^m\right)_{\Gamma_m} + \left(\partial_s \mu^{m+1}, \partial_s \varphi_h\right)_{\Gamma_m} = 0, & \quad \forall \varphi_h \in V^h, \quad (2.4.28a) \\
\left(\mu^{m+1} n^m, \omega_h\right)_{\Gamma_m} - \left([\xi^{m+\frac{1}{2}}]_\perp, \partial_s \omega_h\right)_{\Gamma_m} = 0, & \quad \forall \omega_h \in V^h_0 \times V^h_0, \quad (2.4.28b)
\end{align*}
\]

where the the two contact point positions \(x^c_1(t_{m+1})\) and \(x^c_2(t_{m+1})\) are determined by

\[
\begin{align*}
x^c_1(t_{m+1}) &= x^c_1(t_m) + \tau_m \eta \left[\xi_2^m(n^m_1) - \sigma\right] \quad \text{(2.4.29a)} \\
x^c_2(t_{m+1}) &= x^c_2(t_m) - \tau_m \eta \left[\xi_2^m(n^m_2) - \sigma\right] \quad \text{(2.4.29b)}
\end{align*}
\]

Here \(n^m_j = [n^m_j]_{L_j}\). As in two dimensions, the anisotropy is generally given in the form of \(\gamma(\theta)\) with \(\theta\) representing the angle between the outer normal vector and \(y\) axis. In this case, the Cahn-Hoffman \(\xi\)-vector is given by \(\xi = \gamma(\theta)n + \gamma'(\theta)\tau\). Thus we can define \(\xi^{m+\frac{1}{2}}\) as

\[
\xi^{m+\frac{1}{2}} = \gamma(\theta^m)n^{m+1} + \gamma'(\theta^m)\tau^{m+1}. \quad (2.4.30)
\]
If the anisotropy function is given by a Riemannian metric

$$\gamma(n) = \sum_{l=0}^{L} \sqrt{G_l \cdot n}$$

with $G_l$ a positive definite matrix [19,34], the corresponding Cahn-Hoffman $\xi$-vector is given as

$$\xi(n) = \sum_{l=0}^{L} \left[ \sqrt{G_l \cdot n} \right]^{-1} G_l n,$$

thus we can defined $\xi^{m+\frac{1}{2}}$ as

$$\xi^{m+\frac{1}{2}} = \sum_{l=0}^{L} \left[ \sqrt{G_l m \cdot n^m} \right]^{-1} G_l n^{m+1}.$$ (2.4.32)

In the above numerical scheme, we use the semi-implicit $P_1$-PFEM instead of the fully implicit PFEM such that only a linear system will be solved. All the nonlinear terms have been linearized or explicitly valued. In our practical computation, the linear system is solved either by the GMERES method or the sparse LU decomposition. In addition, it has the following advantages in terms of efficiency: (a) the numerical quadratures are calculated over the curve $\Gamma^m$ instead of $\Gamma^{m+1}$; (b) The nonlinear term $\xi$ is treated technically such that some parts are evaluated on $\Gamma^m$ and the other parts are evaluated on $\Gamma^{m+1}$. Thus it is much more efficient than the fully implicit PFEM.

We have the following theorem for the PFEM scheme:

**Theorem 2.4.1** (Well-posedness for the PFEM scheme). The discrete variational problem Eqs. (2.4.28a),(2.4.28b),(2.4.29a) and (2.4.29b) is well-posed.

**Proof.** Note the two contact points is updated explicitly and can be consider as Dirichlet boundary conditions. To prove that the linear system has the unique solution is equivalent to prove that the corresponding homogeneous linear system has zero solution. Here we only show the case when the anisotropy is given by $\gamma(\theta)$, since the proof of the anisotropy in Riemannian metric form has already been presented in [19]. The homogeneous system can be reduced to: find $\{X^{m+1}, \mu^{m+1}\} \in \{V_0^h \times V_0^h, V_h\}$ such that

$$\langle X^{m+1}, \varphi_h n^{m+1} \rangle_{\Gamma_m} + \tau_m \langle \partial_s \mu^{m+1}, \partial_s \varphi_h \rangle_{\Gamma_m} = 0, \ \forall \varphi_h \in V_h,$$ (2.4.33a)

$$\langle \mu^{m+1} n^m, \omega_h \rangle_{\Gamma_m} - \langle \xi^{m+\frac{1}{2}} \perp, \partial_s \omega_h \rangle_{\Gamma_m} = 0, \ \forall \omega_h \in V_0^h \times V_0^h.$$ (2.4.33b)
with \( \xi^{m+\frac{1}{2}} = \gamma(\theta^m)[-\partial_sX^{m+1}]^\bot + \gamma'(\theta^m)\partial_sX^{m+1} \). Now take \( \varphi_h = \mu^{m+1}, \omega_h = X^{m+1} \).

By noting that \( [\partial_sX^{m+1}]^\bot \cdot \partial_sX^{m+1} = 0 \), we obtain

\[
\tau_m \left< \partial_s\mu^{m+1}, \partial_s\mu^{m+1} \right>_g^h + \left< \gamma(\theta^m)\partial_sX^{m+1}, \partial_sX^{m+1} \right>_g^h = 0. \tag{2.4.34}
\]

This directly gives us that \( X^{m+1} = 0, \mu^{m+1} = 0 \). Thus the corresponding homogeneous linear system only has zero solution, which indicates our discrete scheme has unique solution.

To summarise, our PFEM scheme shows many advantages over the PFEM scheme proposed in [8]. In [8], (a) it needs to calculate the second derivative of the anisotropy \( \gamma(\theta) \) while our scheme only needs the first derivative of the anisotropy. (b) It includes another variational equation relating to the curvature and our scheme seems much simpler. (c) The well-posedness for the scheme is only established when the surface energy is isotropic while the well-posedness our scheme can be proved for a more general class of anisotropies. In the above numerical scheme, initially at \( t = t_0 = 0 \), we can always choose \( \Gamma^0 = X^0 \in V^h_{x(0),x(0)} \times V^h_{x(0)} \) such that the mesh points \( \{X^0(\rho_j)\}_{j=1}^N \) are equally distributed with respect to the arc length \( s \). Certainly, when \( m \geq 1 \), the partition points on \( \Gamma^m \) might be no longer equally distributed with respect to the arc length \( s \). In order to track the mesh quality in real time, we define the mesh-distribution function as

\[
\Psi(t = t_m) = \Psi^m \equiv \frac{\max_{1 \leq j \leq N} ||X^m(\rho_j) - X^m(\rho_{j-1})||}{\min_{1 \leq j \leq N} ||X^m(\rho_j) - X^m(\rho_{j-1})||}
\]

at the time level \( t_m \). If \( \Psi^m \) becomes too large, the excessive uneven distribution mesh will severely contaminate the numerical scheme and make it become unstable. In order to overcome the problem, we need to redistribute the mesh points when the strength parameter \( \Psi^m \) is larger than a prescribed critical value. The mesh redistribution procedure is as follows: (i) given the coordinates \((x, y)\) of the mesh points at the time, a piecewise linear curve can be obtained by using linear fittings for every two consecutive points; (ii) we can obtain the arc length between any two consecutive points, and therefore the total arc length; and (iii) according to these arc lengths and linear polynomials, we redistribute these mesh points at evenly spaced arc lengths. Another mesh distribution algorithm which conserves the total area...
2.4 A parametric finite element method (PFEM)

is given in a form of Gauss-Seidel type iteration in [6]. This algorithm is useful in three dimension mesh regularization but too costly for the regularization of a two dimensional curve as our mesh distribution method is proved to be good enough in practice. On the other hand, this actually might not bring pronounced disadvantages for the numerical scheme as the anisotropy is isotropic or near isotropic, we can observe that the $\Psi^m \to 1$ when $m \to \infty$. This long-time equi-distribution property has been discussed in the PFEM [16].

Our scheme mainly focus on the linearization of the nonlinear term $\xi$-vector. Two kinds of expressions for $\xi$-vector are given for two kinds of anisotropies. Yet, there is not stability result for our PFEM scheme for the first case when the anisotropy is given by $\gamma(\theta)$. In addition, the stability bound in the second case when the anisotropy is in the form of Riemannian metric is given by J.W. Barrett in [19], but only for closed curves with periodical boundary conditions. Therefore, we need a more generalized PFEM scheme which can overcome these drawbacks and are applicable for all types of anisotropies. Based on the work done by Deckelnick [35,36] on graphs, here we can propose another discrete scheme such that the nonlinear term $\xi$ is explicitly valued by adding a stabilized term on the right hand side. The scheme can be given as: for $m \geq 0$, find $\Gamma^{m+1} = X^{m+1} \in V^h_{a,b} \times V^h_0$ with the $x$-coordinate positions of the moving contact points $a := x^l(t_{m+1}) \leq b := x^r(t_{m+1})$ and $\mu^{m+1} \in V^h$ such that

$$\frac{X^{m+1} - X^m}{\tau_m}, \varphi_h n^m \bigg\rangle_{\Gamma^m}^h + \bigg\langle \partial_s \mu^{m+1}, \partial_s \varphi_h \bigg\rangle_{\Gamma^m}^h = 0, \quad \forall \varphi_h \in V^h, \quad (2.4.35a)$$

$$\bigg\langle \mu^{m+1} n^m, \omega_h \bigg\rangle_{\Gamma^m}^h - \bigg\langle [\xi^m]^\perp, \partial_s \omega_h \bigg\rangle_{\Gamma^m}^h - \lambda \big(\gamma(n^m) \partial_s (X^{m+1} - X^m), \partial_s \omega_h \big)_{\Gamma^m}^h = 0, \quad \forall \omega_h \in V^h_0 \times V^h_0, \quad (2.4.35b)$$

where the two contact point positions $x^l(t_{m+1})$ and $x^r(t_{m+1})$ are determined by Eqs. (2.4.29a),(2.4.29b). Here $\lambda$ is positive and related to $\gamma$.

The stability result for scheme (2.4.35a) and (2.4.35b) with periodical boundary conditions can be established and the proof is quite similar to the work in [36], so we omit the proof. Since the stabilized parameter will highly influence the accuracy
of the scheme, especially when $\lambda$ is in the magnitude of $1/\delta t$, so this scheme is not our first option compared to the former PFEM scheme.

2.5 Numerical results

Based on the mathematical model and numerical methods presented above, we will test the convergence order of our PFEM Eqs. (2.4.28a),(2.4.28b),(2.4.29a) and (2.4.29b). For comparison, the convergence order of PFEM for closed curve (periodical boundary conditions) will also be presented. In addition, we will present the numerical simulation results in this section from simulating solid-state dewetting in several different thin-film geometries with several kinds of anisotropic surface energy in 2D. For simplicity, we set the initial thin film thickness to unity in the following simulations. The contact line mobility $\eta$ determines the relaxation rate of the dynamical contact angle to the equilibrium contact angle, and in principle, it is a material parameter and should be determined either from physical experiments or microscopic (e.g., molecular dynamical) simulations. Here we will always choose the contact line mobility as $\eta = 100$ in numerical simulations, and the detailed discussion about its influence to solid-state dewetting evolution process can be found in the reference [120]. The first kind of anisotropic surface energy density we consider is the $k$-fold crystalline surface energy

$$\gamma(\theta) = 1 + \beta \cos[k(\theta + \phi)], \quad \theta \in [-\pi, \pi],$$

(2.5.1)

where $\beta \geq 0$ controls the degree of the anisotropy, $k$ is the order of the rotational symmetry (usually taken as $k = 2, 3, 4, 6$ for crystalline materials and $\phi \in [0, \pi]$ represents a phase shift angle describing a rotation of the crystallographic axes of the thin film with respect to the substrate plane. In this section we only focus on the weakly anisotropic case $0 \leq \beta < \frac{1}{k^2 - 1}$. Another type of surface energy density which has been discussed in [19], is presented in the Riemannian metric,

$$\gamma(n) = \sum_{l=0}^{L} \sqrt{R(-\phi_l)D(\delta_l)R(\phi_l)n \cdot n},$$

(2.5.2)
where
\[
D(\delta_l) = \begin{pmatrix} 1 & 0 \\ 0 & \delta_l^2 \end{pmatrix}, \quad R(\phi) = \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix}.
\]
(2.5.3)

Here the matrix \( D \) is regularized to be positive definite.

### 2.5.1 Convergence test

Firstly we apply our PFEM on the closed curve evolution and open curve evolution (solid-state dewetting problem) under surface diffusion both in isotropic and weakly anisotropic cases. The uniform time step is used during the numerical simulation.

For closed curve evolution, including the isotropic (shown in Table 2.1) and anisotropic (shown in Table 2.2) cases, the initial shape of thin film is chosen as a closed tube, i.e., a rectangle of length 4 and width 1 added by two semi-circles with radii of 0.5 to its left and right sides, and the parameters \( h_0 = (8 + \pi)/120 \) and \( \tau_0 = 0.01 \); for an open curve evolution, including the isotropic (shown in Table 2.3) and anisotropic (shown in Table 2.4) cases, the initial shape of thin film is chosen as a rectangle island of length 5 and thickness 1, and \( h_0 = 0.05 \) and \( \tau_0 = 0.005 \).

In order to compute the convergence order at any fixed time, we can define the following numerical approximation solution in any time interval as
\[
X_{h,\tau}(\rho_j, t) = \frac{t - t_{m-1}}{\tau} X^m(\rho_j) + \frac{t_{m-1} - t}{\tau} X^{m-1}(\rho_j), \quad j = 0, 1, \ldots, N, t \in [t_{m-1}, t_m],
\]
(2.5.4)

where \( h \) and \( \tau \) denote the uniform grid size and time step that we used in the numerical simulations. The numerical error \( e_{h,\tau}(t) \) in the \( L^\infty \) norm can be defined as
\[
e_{h,\tau}(t) = \| X_{h,\tau} - X_{h,\tau}^\tau \|_{L^\infty} = \max_{0 \leq j \leq N} \min_{\rho \in [0,1]} |X_{h,\tau}(\rho_j, t) - X_{h,\tau}^\tau(\rho, t)|,
\]
(2.5.5)

where the curve \( X_{h,\tau}^\tau(\rho, t) \) belongs to the piecewise linear finite element vector spaces and at the interval nodes \( \rho = \rho_j \), its values are equal to the values of numerical solutions \( X_{h,\tau}^\tau(\rho_j, t) \).
### 2.5 Numerical results

Table 2.1: Convergence rates in the $L^\infty$ norm for a closed curve evolution under the isotropic surface diffusion flow, that is the surface energy density $\gamma = 1$

<table>
<thead>
<tr>
<th>$e_{h,\tau}(t)$</th>
<th>$h = h_0$</th>
<th>$h_0/2$</th>
<th>$h_0/2^2$</th>
<th>$h_0/2^3$</th>
<th>$h_0/2^4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau = \tau_0$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 0.5)$</td>
<td>4.58E-3</td>
<td>1.09E-3</td>
<td>2.63E-4</td>
<td>6.40E-5</td>
<td>1.58E-5</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>2.07</td>
<td>2.05</td>
<td>2.04</td>
<td>2.02</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 2.0)$</td>
<td>3.61E-3</td>
<td>9.43E-4</td>
<td>2.45E-4</td>
<td>6.31E-5</td>
<td>1.61E-5</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>1.94</td>
<td>1.95</td>
<td>1.96</td>
<td>1.97</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 5.0)$</td>
<td>3.63E-3</td>
<td>9.47E-4</td>
<td>2.46E-4</td>
<td>6.33E-5</td>
<td>1.62E-5</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>1.94</td>
<td>1.95</td>
<td>1.96</td>
<td>1.97</td>
</tr>
</tbody>
</table>

Table 2.2: Convergence rates in the $L^\infty$ norm for a closed curve evolution under the anisotropic surface diffusion flow, where $\gamma(\theta) = 1 + 0.05\cos(4\theta)$

<table>
<thead>
<tr>
<th>$e_{h,\tau}(t)$</th>
<th>$h = h_0$</th>
<th>$h_0/2$</th>
<th>$h_0/2^2$</th>
<th>$h_0/2^3$</th>
<th>$h_0/2^4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau = \tau_0$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 0.5)$</td>
<td>1.24E-2</td>
<td>2.25E-3</td>
<td>6.71E-4</td>
<td>2.48E-4</td>
<td>7.10E-5</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>2.46</td>
<td>1.74</td>
<td>1.44</td>
<td>1.80</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 2.0)$</td>
<td>4.86E-3</td>
<td>1.44E-3</td>
<td>4.57E-4</td>
<td>1.37E-4</td>
<td>3.71E-5</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>1.76</td>
<td>1.66</td>
<td>1.74</td>
<td>1.89</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 5.0)$</td>
<td>4.88E-3</td>
<td>1.44E-3</td>
<td>4.58E-4</td>
<td>1.37E-5</td>
<td>3.74E-5</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>1.76</td>
<td>1.66</td>
<td>1.74</td>
<td>1.89</td>
</tr>
</tbody>
</table>
2.5 Numerical results

Table 2.3: Convergence rates in the $L^\infty$ norm for an open curve evolution under the isotropic surface diffusion flow (solid-state dewetting with isotropic surface energy), where $\gamma(\theta) = 1, \sigma = \cos(5\pi/6)$.

<table>
<thead>
<tr>
<th>$e_{h,\tau}(t)$</th>
<th>$h = h_0/2^0$</th>
<th>$h_0/2$</th>
<th>$h_0/2^2$</th>
<th>$h_0/2^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e_{h,\tau}(t = 0.5)$</td>
<td>2.59E-2</td>
<td>1.32E-2</td>
<td>6.52E-3</td>
<td>3.29E-3</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>0.97</td>
<td>1.01</td>
<td>0.99</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 2.0)$</td>
<td>2.39E-2</td>
<td>1.22E-2</td>
<td>6.10E-3</td>
<td>3.07E-3</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>0.97</td>
<td>1.00</td>
<td>0.99</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 5.0)$</td>
<td>1.91E-2</td>
<td>9.67E-3</td>
<td>4.84E-3</td>
<td>2.43E-3</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>0.98</td>
<td>1.00</td>
<td>0.99</td>
</tr>
</tbody>
</table>

Table 2.4: Convergence rates in the $L^\infty$ norm for an open curve evolution under the anisotropic surface diffusion flow (solid-state dewetting with anisotropic surface energy), where $\gamma(\theta) = 1 + 0.05 \cos(4\theta), \sigma = \cos(5\pi/6)$.

<table>
<thead>
<tr>
<th>$e_{h,\tau}(t)$</th>
<th>$h = h_0/2^0$</th>
<th>$h_0/2$</th>
<th>$h_0/2^2$</th>
<th>$h_0/2^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e_{h,\tau}(t = 0.5)$</td>
<td>2.82E-2</td>
<td>1.41E-2</td>
<td>6.88E-3</td>
<td>3.44E-3</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>0.99</td>
<td>1.04</td>
<td>1.00</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 2.0)$</td>
<td>2.71E-2</td>
<td>1.37E-2</td>
<td>6.78E-3</td>
<td>3.40E-3</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>0.98</td>
<td>1.02</td>
<td>0.99</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 5.0)$</td>
<td>2.32E-2</td>
<td>1.12E-3</td>
<td>5.80E-3</td>
<td>2.92E-3</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>1.00</td>
<td>1.00</td>
<td>0.99</td>
</tr>
</tbody>
</table>
2.5 Numerical results

We compute the convergence rate of the scheme at three different times \( t = 0.5, t = 2.0, t = 5.0 \). The results are shown in Table. 2.1-2.4. From the table, we can clearly observe that for closed curve evolution under surface diffusion, the convergence order is second order when the surface energy is isotropic. However, the anisotropic surface energy can decrease the convergence order to around 1.7 (Table. 2.2). This deterioration may be caused by the linearization of \( \xi (\xi^{m+\frac{1}{2}} = \gamma (\theta^m)(-\partial_s X^{m+1}) - \gamma' (\theta^m) \partial_s X^{m+1}) \). For the open curves, the convergence order further reduce to first order both for the isotropic and anisotropic cases. This deterioration may be due to that the forward Euler scheme was applied to discretize the relaxed contact angle boundary condition, i.e. Eq. (2.3.8).

Compared to the traditional explicit finite difference method (e.g., marker-particle methods) for computing the fourth-order geometric evolution PDEs [42, 120, 125], which imposes the extremely strong stability restriction on the time step, i.e., \( \tau \sim O(h^4) \), the proposed semi-implicit PFEM can greatly alleviate the stability restriction and our numerical experiments indicate that the time step only needs to be chosen as \( \tau \sim O(h^2) \) to maintain the numerical stability. Of course, rigorous numerical analysis for these observations including convergence rates and stability condition of PFEM is very important and challenging, while its mathematical study is ongoing.

2.5.2 Small islands

In the following, we show some numerical simulations of solid-state dewetting with isotropic/weakly anisotropic surface energy. Fig. 2.2 shows the evolution of an initial rectangle thin film (red solid line) with length 5 and height 1 towards its equilibrium (blue solid line) under the 4-fold anisotropy (see Eq. (2.5.1) with \( k = 4 \)). For Fig. 2.2(a) to Fig. 2.2(d), the material constant is all chosen \( \sigma = \cos(\frac{3\pi}{4}) \), while the degree \( \beta \) of the anisotropy is increased gradually \( \beta = 0 \) to \( \beta = 0.06 \). As can be seen clearly in the figure, the corresponding equilibrium shapes changes from a part of a circle (isotropy) to a anisotropic shape with increasingly sharper corner. The
Figure 2.2: Several steps in the evolution of small, initial rectangle islands (shown in red) towards their equilibrium shapes (shown in blue) for different degrees of the anisotropy $\beta$ with the crystalline symmetry order $k = 4$. The material constant is chosen as $\sigma = \cos \frac{3\pi}{4}$. And for each figure (a) $\beta = 0$, (b) $\beta = 0.02$, (c) $\beta = 0.04$, (d) $\beta = 0.06$. 
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Figure 2.3: Several steps in the evolution of small initial rectangle islands (shown in red) towards their equilibrium shape (shown in blue) with $\gamma(\theta) = 1 + \beta \cos(k\theta), \sigma = \cos \frac{3\pi}{4}$. (a) $k = 3, \beta = 0.1$; (b) $k = 6, \beta = 0.022$.

Figure 2.4: (a) The temporal evolution of the normalized free energy and normalized mass, (b) the temporal evolution of the mesh distribution function $\psi(t)$. The computational parameters are chosen as same as Fig. 2.2(c).
numbers of ”facets” in the equilibrium shape exhibits the 4− fold symmetry. The $k$-fold symmetry effect can also be observed in Fig. 2.3 with $k = 3$ and $k = 6$.

Fig. 2.4(a) shows the temporal evolution of the normalized free energy $W(t)/W(0)$ and normalized area $A(t)/A(0)$ defined in previously while Fig. 2.4(b) shows the temporal evolution of the mesh distribution function $\psi(t)$. The horizontal black dash line in the figure demonstrates that our discrete scheme has a good property of maintaining the total area. The monotonically decreasing red solid line implies the energy dissipation during the entire simulations. For the mesh distribution function, we can observe it first increase to 3 and then gradually decrease to a value around 2, which implies that the mesh is preserved well during our simulation for the $k$-fold anisotropy when the degree $\beta$ is not big enough.

![Figure 2.5](image_url)

Figure 2.5: Equilibrium island morphologies for a small, initially rectangular island film under several different crystalline rotations $\phi$ (phase shifts): (a) $\phi = 0$; (b) $\phi = \pi/6$; (c) $\phi = \pi/4$; (d) $\phi = \pi/3$. The other computational parameters are chosen as: $k = 4, \beta = 0.06, \sigma = \cos(5\pi/6)$.

To observe rotation effects of the crystalline axis of the island relative to the substrate normal, we also performed numerical simulations of the evolution of small
2.5 Numerical results

Figure 2.6: Several steps in the evolution of small, initially rectangular island (shown in red) towards their equilibrium shapes (shown in blue) where the anisotropy is given by Eq. (2.5.2), \( \sigma = \frac{3\pi}{4} \) with (a) \( L = 1, \phi_0 = 0, \phi_1 = \frac{\pi}{2}, \delta_0 = \delta_1 = 0.1 \) (b) \( L = 2, \phi_0 = 0, \phi_1 = \frac{\pi}{3}, \phi_2 = \frac{2\pi}{3}, \delta_0 = \delta_1 = \delta_2 = 0.1 \).

Figure 2.7: The temporal evolution of the normalized free energy and normalized mass, where the anisotropy is given by Eq. (2.5.2). The computational parameters are chosen as same as Fig. 2.6(a).
islands with different phase shifts $\phi$ for the weakly anisotropic cases under the computational parameters: $k = 4, \beta = 0.06, \sigma = \cos(5\pi/6)$. As shown in Fig. 2.5, the asymmetry of the equilibrium shapes is clearly observed, which can be explained as breaking the symmetry of the surface energy anisotropy (defined in Eq. (2.5.1)) with respect to the substrate normal.

Figure 2.8: Several snapshots in the evolution of a small, initially rectangular island film towards its equilibrium shape: (a) $t = 0$; (b) $t = 0.1$; (c) $t = 0.6$; (d) $t = 7.5$. The anisotropy is chosen $\gamma(\theta) = 1 + 0.19|\cos(\frac{5\pi}{6}\theta)|$ with smooth regularization parameter $\delta = 0.1$. The computational parameter is chosen as $\sigma = \cos(3\pi/4), \lambda = 20$.

Fig. 2.6 shows the dynamic evolution a small initial island (red solid line) towards its equilibrium shape (blue solid line) under the anisotropy which is given by Eq. (2.5.2). For Fig. 2.6(a),(b), the material constant is chosen as $\sigma = \cos(\frac{3\pi}{4})$, while the parameter that determines the anisotropy is chosen as following: (a) $L = 1, \phi_0 = 0, \phi_1 = \frac{\pi}{2}, \delta_0 = \delta_1 = 0.1$ and (b) $L = 2, \phi_0 = 0, \phi_1 = \frac{\pi}{3}, \phi_2 = \frac{2\pi}{3}, \delta_0 = \delta_1 = \delta_2 = 0.1$. We can clearly see that the equilibrium shapes for this type of anisotropy have
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sharper corners than the $k$-fold anisotropy. The equilibrium shape for (a) is a truncation of a square and (b) a truncation of a hexagon, which implies that $L$ play the same roles in determining the symmetry as $k$ does in the $k$-fold anisotropy. The small parameter $\delta$ is used to smoothen the surface energy density function, which in the equilibrium shape can be explained to smooth the sharp corners. Fig. 2.7 shows the temporal evolution of the normalized free energy $W(t)/W(0)$ and normalized mass $A(t)/A(0)$. It clearly indicates that our discrete scheme has the same good properties of maintaining mass conservation and energy dissipation under this cusps surface energy density. The last anisotropy we consider is given by

$$\gamma(\theta) = 1 + \beta|\cos(k/2^\theta)|. \quad (2.5.6)$$

This anisotropy is not smooth at the point where $\cos(k/2^\theta)$ changes its sign. A smooth regularization is necessary

$$\gamma(\theta) = 1 + \beta \sqrt{\delta^2 + \cos^2(k/2^\theta)}. \quad (2.5.7)$$

Numerical simulations indicate that our PFEM scheme (2.4.28a)-(2.4.29b) is not working well for this type anisotropy. So we apply the stabilized PFEM scheme (2.4.35a), (2.4.35b) for this special case. Fig. 2.8 shows the evolution of a small rectangular island towards its equilibrium shape with this anisotropy chosen as $\gamma(\theta) = 1 + 0.19|\cos(5/2^\theta)|$. From the figure, we can observe that the equilibrium is almost a truncation of pentagon, which indicates that $k$ represents the rotational symmetry.

2.5.3 Large islands

As noted in the papers [8, 40, 66, 120], when the aspect ratios of thin island films are larger than a critical value, the islands will pinch-off. Fig. 2.9 depicts the temporal evolution of a very large island film (aspect ratio of 60) with weakly anisotropic surface energy. As shown in Fig. 2.9, solid-state dewetting very quickly leads to the formation of ridges at the island edges followed by valleys. As time
2.5 Numerical results

Figure 2.9: Several snapshots in the evolution of a long, thin island film (aspect ratio of 60) with \( k \)-fold anisotropic surface energy \( (k = 4, \beta = 0.06, \phi = 0) \) and the material parameter \( \sigma = \cos(5\pi/6) \). (a) \( t = 0 \); (b) \( t = 10 \); (c) \( t = 240 \); (d) \( t = 320 \); (e) \( t = 371 \); (f) \( t = 711 \). Note the difference in vertical and horizontal scales.

Figure 2.10: The corresponding temporal evolution in Fig. 2.9 for the normalized total free energy and the normalized area (mass).
Figure 2.11: Several snapshots in the evolution of a long, thin island film (aspect ratio of 40) for surface energy defined in (2.5.2), with $L = 1, \phi_0 = \pi/4, \phi_1 = 3\pi/4, \delta_0 = \delta_1 = 0.1$. The material parameter is chosen as $\sigma = \cos(5\pi/6)$: (a) $t = 0$; (b) $t = 10$; (c) $t = 50$; (d) $t = 100$; (e) $t = 140$; (f) $t = 400$. Note the difference in vertical and horizontal scales.
2.5 Numerical results

evolves, the ridges and valleys become increasingly exaggerated, then the two valleys merge near the island center. At the time $t = 371$, the valley at the center of the island hits the substrate, leading to a pinch-off event that separates the initial island into a pair of islands. Finally, the two separated islands continue to evolve until they reach their equilibrium shapes. The corresponding evolution of the normalized total free energy and normalized total area (mass) are shown in Fig. 2.10. An interesting phenomenon here is that the total energy undergoes a sharp drop at $t = 371$, the moment when the pinch-off event occurs. In order to obtain a qualitative comparison with other methods, we choose the same computational parameters as in the paper [120]. The pinch-off time $t = 371$ we obtained by using our PFEM for this example is very close to the result $t = 374$ by using marker-particle methods in [120]. But under the same computational resource, the computational time by using PFEM for this example is about several hours, while it is about two weeks by using marker-particle methods [120]. Besides, the pinch-off time is exactly the same to the result by using another PFEM method in [8], which validates the accuracy of our PFEM. Note here that once the interface curve hits the substrate somewhere in the simulation, it means that a pinch-off event has happened and a new contact point is generated, then after the pinch-off, we compute each part of the pinch-off curve separately.

The pinch-off can also be observed for the surface energy defined in Eq. (2.5.2). Fig. 2.11 shows the evolution of a large, initially rectangular islands with aspect ratio of 40. with material constant $\sigma$ same as Fig. 2.9. The parameters that determine the surface energy are chosen as $L = 1, \phi_0 = \pi/4, \phi_0 = 3\pi/4, \delta_0 = \delta_1 = 0.1$. From the figure we can observe that the thin film form valleys and ridges at the edge and then pinch-off happens at time $t = 140$. The thin film breaks up into two small thin islands which later evolve into the equilibrium shapes.
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2.5.4 Semi-infinite films

For semi-infinite film, a lot of earlier studies [66, 70, 111, 125] have shown that the retraction distance of a solid-thin film scales with time according to a power-law relation such that \( R(t) \sim t^\alpha \) and \( \alpha \approx \frac{3}{5} \). The retraction power law exponent \( \alpha \) can vary with different anisotropies and material parameters. So here we want to investigate this power law pattern by performing numerical simulations on the semi-infinite thin film with cusps surface energy (Eq. (2.5.2)). See Fig. 2.12 and Fig. 2.13, the initial film is chosen with height 1. The parameter for Fig. 2.12 is chosen as \( \sigma = \cos \frac{5\pi}{6}, L = 2, (\phi_1, \phi_2) = (0, \frac{\pi}{2}), \delta_1 = \delta_2 = 0.1 \). The parameter for Fig. 2.13 is the same except \( (\phi_1, \phi_2) = (\frac{\pi}{4}, \frac{3\pi}{4}) \). It can be seen clearly, in Fig. 2.12, the left contact point moves gradually towards \(+x\) direction, but no valley and ridge are formed on the surface of the thin film. The thin film stays rectangular shape during the evolution, thus it is very hard for the thin film to pinch off. This phenomenon could be explained by considering how the thin film tends to lower the surface energy. As the surface energy density obtain its minimum at the orientation \( \mathbf{n} = (0, 1)^T, (1, 0)^T, (-1, 0)^T \), then the thin film will stay rectangular shape without formation of ridges and valleys. On the contrary, if a rotation is forced on the surface energy density, see in Fig. 2.13, the edge of the thin film retract towards \(+x\) direction and the valley is formed quickly. Therefore, a small thin film quickly break up from the whole film in a short time (see Fig. 2.13(e), a small thin film breaks up from the whole film at time \( t = 445 \)).

Fig. 2.14 and Fig. 2.15 are the loglog plots of the retraction distance \( R(t) \) versus the time \( t \) for different \( \sigma \). For Fig. 2.14, the anisotropy is chosen the same as Fig. 2.12 with \( (\phi_1, \phi_2) = (0, \frac{\pi}{2}) \), while for Fig. 2.15, the anisotropy is chosen the same as Fig. 2.13. The numerical simulations clearly demonstrate that the retraction distance \( R(t) \) satisfies the power law with the exponent \( \alpha \approx 0.4 \) in these two cases. Fig. 2.16 shows the numerical fitting result of the the power law exponent \( \alpha \) for different \( \sigma \) in the two cases. From the figure, we can see the exponent \( \alpha \) can depend on the material constant \( \sigma \). Since from Fig. 2.14, we can observe that as \( \sigma \) become
2.5 Numerical results

\[ \sigma = \cos\left(\frac{5\pi}{6}\right), \gamma \text{ is chosen as Eq. (2.5.2) with } L = 2; \phi = (0, \frac{\pi}{2}), \delta_1 = \delta_2 = 0.1, \text{ where} \]

(a) \( t = 0 \); (b) \( t = 10 \); (c) \( t = 100 \); (d) \( t = 500 \); (e) \( t = 2500 \).

Figure 2.12: The evolution of semi infinite long film with parameter chosen as: \( \sigma = \cos\left(\frac{5\pi}{6}\right), \gamma \text{ is chosen as Eq. (2.5.2) with } L = 2; \phi = (0, \frac{\pi}{2}), \delta_1 = \delta_2 = 0.1, \text{ where} \)

(a) \( t = 0 \); (b) \( t = 10 \); (c) \( t = 100 \); (d) \( t = 200 \); (e) \( t = 445 \).

\[ \sigma = \cos\left(\frac{5\pi}{6}\right), \gamma \text{ is chosen as Eq. (2.5.2) with } L = 2; \phi = (\frac{\pi}{4}, \frac{3\pi}{4}), \delta_1 = \delta_2 = 0.1, \text{ where} \]

(a) \( t = 0 \); (b) \( t = 10 \); (c) \( t = 100 \); (d) \( t = 200 \); (e) \( t = 445 \).
2.5 Numerical results

Figure 2.14: The retraction distance versus the time $t$ for different $\sigma$, where $\phi = (0, \frac{\pi}{2})$.

Figure 2.15: The retraction distance versus the time $t$ for different $\sigma$ till the pinch off happening, where $\phi = (\frac{\pi}{4}, \frac{3\pi}{4})$.
smaller, the retraction distance are more easier to become linear. For $\sigma = 1.0$, it still takes a much longer time for the retraction distance obtain the power law in this case. So this could help explain that why fitting exponent is much larger than expected for $\sigma = 1.0$ in the first case.

2.6 Extension to strongly anisotropic case

In 2D, a sharp corner could exist in the equilibrium shape when the surface stiffness $H, (n) \tau \cdot \tau \leq 0$ for some $\tau \in S^1$. Thus the surface diffusion problem induced from the free energy functional is not well-posed. The approach to treating this ill-posed problem is to add a high-order term to the total surface energy. In this section, we will follow the approach in [57, 80] and regularize the problem with the Willmore energy, which is given by

$$W_\tau = \frac{\sigma^2}{2} \int_\Gamma \kappa^2 \, ds,$$

(2.6.1)
where \( \kappa \) is curvature of the curve and \( \delta \) is a small regularization parameter. With this regularization, the dimensionless total energy can be written as follows

\[
W_{\text{reg}}^{\delta} = W + W_r = \int_{\Gamma} (\gamma(n) + \frac{\delta^2}{2} \kappa^2) \, ds - \sigma(x_r - x_c^l). \tag{2.6.2}
\]

### 2.6.1 The regularized energy and thermodynamic variation

In order to perform the first variation of the total surface energy defined in Eq. (2.6.2), we need the following lemma.

**Lemma 2.6.1.** Suppose \( \Gamma = X(s) \in C^4([0, L]) \times C^4([0, L]) \) is an open curve where \( s(0 \leq s \leq L) \) is the arc length. Consider a perturbation for \( \Gamma \) with \( V(\rho, \varepsilon) \) representing the smooth variational vector field defined in Eq. (2.1.4). Let \( F(\Gamma) = \int_{\Gamma} \kappa^2 \, ds \), then we have

\[
dF(\Gamma; V) = -\int_{\Gamma} (\kappa^3 + 2\partial_s \kappa)(n \cdot V_0) \, ds
- \left(2\kappa n \cdot \partial_s V_0 - 2\partial_s \kappa (n \cdot V_0) + \kappa^2 (\tau \cdot V_0)\right)\bigg|_{s=L}^{s=0}. \tag{2.6.3}
\]

**Proof.** If we define \( \theta^\varepsilon = \theta(\rho, \varepsilon) = \arctan \frac{\partial_{x^2}(\rho, \varepsilon)}{\partial_{x^1}(\rho, \varepsilon)} \), then \( \kappa \) can be expressed as

\[
\kappa^\varepsilon = -\partial_s \theta^\varepsilon = -\frac{\partial_{\rho} X(\rho, \varepsilon)}{|\partial_{\rho} X(\rho, \varepsilon)|}. \tag{2.6.4}
\]

From the parameterization defined in Eq. (2.1.3), \( F(\Gamma^\varepsilon) \) is given by

\[
F(\Gamma^\varepsilon) = \int_0^1 (\kappa^\varepsilon)^2 |\partial_{\rho} X(\rho, \varepsilon)| \, d\rho. \tag{2.6.5}
\]

By taking derivative of \( F(\Gamma^\varepsilon) \) with respect to \( \varepsilon \) and noting the independence between \( \varepsilon \) and \( \rho \), based on Eq. (2.6.4), we have

\[
\frac{d}{d\varepsilon} F(\Gamma^\varepsilon) = \int_0^1 2\kappa^\varepsilon \partial_{\theta^\varepsilon} \partial_{\rho} X(\rho, \varepsilon) |\partial_{\rho} X(\rho, \varepsilon)| \, d\rho + \int_0^1 (\kappa^\varepsilon)^2 \partial_s |\partial_{\rho} X(\rho, \varepsilon)| \, d\rho
= -2 \int_0^1 \kappa^\varepsilon \partial_s \partial_{\rho} \theta^\varepsilon \, d\rho - 2 \int_0^1 \kappa \partial_{\theta^\varepsilon} \partial_s \frac{1}{|\partial_{\rho} X(\rho, \varepsilon)|} \partial_{\rho} X(\rho, \varepsilon) \, d\rho
+ \int_0^1 \kappa^2 \partial_s \partial_{\rho} X(\rho, \varepsilon) \, d\rho
= I + II + III. \tag{2.6.6}
\]
Note that the expansion of $\theta^\varepsilon$ and $\frac{1}{|\partial_p X(\rho, \varepsilon)|}$ at $\varepsilon = 0$ give us

\[
\theta^\varepsilon = \theta - \frac{\partial_p X^\perp \cdot \partial_p V_0}{|\partial_p X|^2} \varepsilon + O(\varepsilon^2) = \theta + \theta' \varepsilon + O(\varepsilon^2).
\]

(2.6.7a)

\[
\frac{1}{|\partial_p X(\rho, \varepsilon)|} = \frac{1}{|\partial_p X|} - \frac{\partial_p X \cdot \partial_p V_0}{|\partial_p X|^3} \varepsilon + O(\varepsilon^2).
\]

(2.6.7b)

Using above expansion and Eq. (2.1.10a), and for the three parts $I$, taking value at $\varepsilon = 0$ and then integration by parts, we have

\[
I \bigg|_{\varepsilon=0} = \int_0^1 2\kappa(-\partial_p \theta') \, d\rho = -\left(2\kappa \theta'\right)_{\rho=0}^1 - \int_0^1 2\partial_p \kappa \left(\frac{\partial_p X^\perp \cdot \partial_p V_0}{|\partial_p X|^2}\right) \, d\rho
\]

\[
= -\left(2\kappa \theta'\right)_{\rho=0}^1 - \int_0^1 2\partial_p \kappa \left(\frac{\partial_p X^\perp \cdot \partial_p V_0}{|\partial_p X|^2}\right) \, d\rho
\]

\[
= -\left(2\kappa \theta'\right)_{\rho=0}^1 - \int_0^1 2\partial_p \kappa \left(\frac{2\partial_p \kappa \partial_p X^\perp}{|\partial_p X|^2}\right) \cdot V_0 \, d\rho
\]

\[
= -\left(2\kappa \theta'\right)_{\rho=0}^1 - \int_0^1 2\partial_p \kappa \left(\frac{2\partial_p \kappa \partial_p X^\perp}{|\partial_p X|^2}\right) \cdot V_0 \, d\rho
\]

\[
= -\left.\left(-2\kappa \theta' + 2\partial_s \kappa \mathbf{n} \cdot \mathbf{V}_0\right)\right|_{s=0}^{s=L} - 2 \int_\Gamma (\partial_s \kappa \mathbf{n} + \partial_s \kappa \kappa \mathbf{V}_0). \quad (2.6.8)
\]

\[
II \bigg|_{\varepsilon=0} = \int_0^1 2\kappa \partial_p \theta \left(\frac{\partial_p X \cdot \partial_p V_0}{|\partial_p X|^2}\right) \, d\rho = 2\left(\kappa \partial_p \theta \left(\frac{\partial_p X \cdot \partial_p V_0}{|\partial_p X|^2}\right)\right)_{\rho=0}^1 - \int_0^1 2\partial_p \left(\kappa \partial_p \theta \left(\frac{\partial_p X}{|\partial_p X|^2}\right)\right) \, d\rho
\]

\[
= 2\left(\kappa \partial_p \theta \left(\frac{\partial_p X \cdot \partial_p V_0}{|\partial_p X|^2}\right)\right)_{\rho=0}^1 + \int_\Gamma 2\kappa \partial_s \left(\frac{2\partial_s \kappa \partial_s X}{|\partial_p X|^2}\right) \cdot \mathbf{V}_0 \, ds
\]

\[
= 2\left(\kappa \partial_p \theta \left(\frac{\partial_p X \cdot \partial_p V_0}{|\partial_p X|^2}\right)\right)_{\rho=0}^1 + \int_\Gamma (4\kappa \partial_s \kappa \partial_s X + 2\partial_s \kappa \partial_s X) \cdot \mathbf{V}_0 \, ds
\]

\[
= -2\left(\kappa^2 \mathbf{\tau} \cdot \mathbf{V}_0\right)_{s=0}^{s=L} + 2 \int_\Gamma (2\kappa^2 \partial_s \kappa \mathbf{\kappa} - \kappa^3 \mathbf{n}) \cdot \mathbf{V}_0 \, ds. \quad (2.6.9)
\]

\[
III \bigg|_{\varepsilon=0} = \int_0^1 \kappa^2 \partial_p \left(\frac{\partial_p X \cdot \partial_p V_0}{|\partial_p X|^2}\right) \, d\rho = \left(\kappa^2 \partial_p \left(\frac{\partial_p X \cdot \partial_p V_0}{|\partial_p X|^2}\right)\right)_{\rho=0}^1 - \int_0^1 \partial_p \left(\kappa^2 \left(\frac{\partial_p X}{|\partial_p X|^2}\right)\right) \, d\rho
\]

\[
= \left(\kappa^2 \partial_p \left(\frac{\partial_p X \cdot \partial_p V_0}{|\partial_p X|^2}\right)\right)_{\rho=0}^1 - \int_\Gamma \partial_s \left(\kappa^2 \partial_s \mathbf{X}\right) \cdot \mathbf{V}_0 \, ds
\]

\[
= \left(\kappa^2 \partial_p \left(\frac{\partial_p X \cdot \partial_p V_0}{|\partial_p X|^2}\right)\right)_{\rho=0}^1 - \int_\Gamma (2\kappa \partial_s \kappa \partial_s X + \kappa^2 \partial_s \mathbf{X}) \cdot \mathbf{V}_0 \, ds
\]

\[
= \left(\kappa^2 \mathbf{\tau} \cdot \mathbf{V}_0\right)_{s=0}^{s=L} - \int_\Gamma (2\kappa \partial_s \kappa \mathbf{\kappa} \mathbf{n} \cdot \mathbf{V}_0 \, ds. \quad (2.6.10)
\]
Summarising them together, so we obtain

\[
dF(\Gamma; V_0) = (I + II + III)\bigg|_{\varepsilon=0} = -\int_\Gamma (\kappa^3 + 2\partial_{ss}\kappa) \mathbf{n} \cdot V_0 \, ds - \left(2\kappa \theta'\right)\bigg|^{s=L}_{s=0} + \left((2\partial_s\kappa \mathbf{n} - \kappa^2 \mathbf{\tau}) \cdot V_0\right)\bigg|^{s=L}_{s=0}.
\]

Note that \(\theta'\) is defined as

\[
\theta' = -\frac{\partial \rho \mathbf{X} \cdot \partial \rho V_0}{|\partial \rho \mathbf{X}|^2} = \mathbf{n} \cdot \partial_s V_0,
\]

thus we have

\[
dF(\Gamma; V_0) = -\int_\Gamma (\kappa^3 + 2\partial_{ss}\kappa) \mathbf{n} \cdot V_0 \, ds - \left(2\kappa \mathbf{n} \cdot \partial_s V_0 - 2\partial_s\kappa (\mathbf{n} \cdot V_0) + \kappa^2 (\mathbf{\tau} \cdot V_0)\right)\bigg|^{s=L}_{s=0}.
\]

Proposition 2.6.1. Suppose \(\Gamma = \mathbf{X}(s) \in C^4([0,L]) \times C^4([0,L])\) is a closed curve where \(s(0 \leq s \leq L)\) is the arc length. Let \(F(\Gamma) = \int_\Gamma \kappa^2 \, ds\), then we have

\[
dF(\Gamma; V) = -\int_\Gamma (\kappa^3 + 2\partial_{ss}\kappa) \mathbf{n} \cdot V_0 \, ds.
\]

Proof. The proof is similar to that of the lemma 2.6.1, but integration by parts will not give us any boundary terms due to the periodic boundary conditions.

\[\Box\]

2.6.2 The regularized model

Now, based on the energy form Eq. (2.6.2), from the lemma. 2.6.1, the first variation of the regularized term is given by

\[
dW_r(\Gamma; V) = -\delta^2 \int_\Gamma (\kappa^3 + \partial_{ss}\kappa) \mathbf{n} \cdot V_0 \, ds + \delta^2 \left(\kappa \mathbf{n} \cdot \partial_s V_0 - \partial_s\kappa (\mathbf{n} \cdot V_0) + \frac{\kappa^2}{2} \mathbf{\tau} \cdot V_0\right)\bigg|^{s=L}_{s=0}.
\]

The boundary term \(-\left(2\kappa \mathbf{n} \cdot \partial_s V_0\right)\bigg|^{s=L}_{s=0}\) inspires us to include the zero curvature boundary conditions into the model to ensure the energy decay for any arbitrary \(\varepsilon\). In addition, the variation vector field is assume to satisfy \((V_x, V_y) = V_0 \parallel \mathbf{x}^+\) on
the boundary. Combined with the Eq. (2.1.14), the first variation of the strongly anisotropic surface energy is given by

$$dW_{\text{reg}}^\delta (\Gamma; \mathbf{V}) = \left[ V_x (\xi_2 - \sigma - \delta^2 n_1 \partial_s \kappa) \right]_{s=L} - \left[ V_x (\xi_2 - \sigma - \delta^2 n_1 \partial_s \kappa) \right]_{s=0} - \int_{\Gamma} (\partial_s \mathbf{x} - \delta^2 \left( \frac{\kappa^3}{2} + \partial_{ss} \kappa \right) \mathbf{n}) \cdot \mathbf{V}_0 \, ds. \quad (2.6.15)$$

Thus we obtain the first variation of the strongly anisotropic surface energy with respect to the curve $\Gamma$ and the two contact points are given as follows

$$\frac{\delta W_{\text{reg}}^\delta}{\delta \Gamma} = - \left[ \partial_s \mathbf{x} \right] \cdot \mathbf{n} - \delta^2 \left( \frac{\kappa^3}{2} + \partial_{ss} \kappa \right), \quad (2.6.16)$$
$$\frac{\delta W_{\text{reg}}^\delta}{\delta x_{lc}^r} = \left[ \xi_2 - \sigma - \delta^2 n_1 \partial_s \kappa \right] \left|_{s=0} \right., \quad (2.6.17)$$
$$\frac{\delta W_{\text{reg}}^\delta}{\delta x_{rc}^r} = \left[ \xi_2 - \sigma - \delta^2 n_1 \partial_s \kappa \right] \left|_{s=L} \right.. \quad (2.6.18)$$

Similar to the case when surface energy density is weak, we can obtain the dimensionless sharp interface model for solid-state dewetting with strongly anisotropic surface energy, which can be written as follows

$$\partial_t \mathbf{X} = \partial_{ss} \mu \, \mathbf{n}, \quad 0 < s < L(t), \quad t > 0, \quad (2.6.19)$$
$$\mu = - \left[ \partial_s \mathbf{x} \right] \cdot \mathbf{n} - \delta^2 \left( \frac{\kappa^3}{2} + \partial_{ss} \kappa \right), \quad \kappa = - (\partial_{ss} \mathbf{X}) \cdot \mathbf{n}; \quad (2.6.20)$$

subject to the following dimensionless boundary conditions:

(i) contact point condition:

$$y(0, t) = 0, \quad y(L, t) = 0, \quad t \geq 0, \quad (2.6.21)$$

(ii) relaxed (or dissipative) contact angle condition:

$$\frac{dx_{lc}^l}{dt} = \eta \left[ \xi_2 - \sigma_0 - \delta^2 \partial_s \kappa n_1 \right] \left|_{s=0} \right., \quad \frac{dx_{rc}^r}{dt} = -\eta \left[ \xi_2 - \sigma_0 - \delta^2 \partial_s \kappa n_1 \right] \left|_{s=L} \right., \quad (2.6.22)$$

(iii) zero-mass flux condition:

$$\partial_s \mu (0, t) = 0, \quad \partial_s \mu (L, t) = 0, \quad t \geq 0, \quad (2.6.23)$$
(iv) zero-curvature condition

\[ \kappa(0, t) = 0, \quad \kappa(L, t) = 0, \quad t \geq 0. \]  \hspace{1cm} (2.6.24)

In the following we will show that the total mass of the thin film is always conserved during the evolution, and the total free energy of the system decreases monotonically at all times.

**Proposition 2.6.2 (Mass conservation and energy dissipation).** Let \( \Gamma(t) = \mathbf{X}(s, t) \) be the exact solution of the Eqs. (2.6.19)-(2.6.20) coupled with boundary conditions Eqs. (2.6.21)-(2.6.24). Given the initial curve \( \Gamma(0) = (x_0(s), y_0(s)) \), then the total mass of the thin film is conserved during the evolution, i.e.,

\[ A(t) \equiv A(0) = \int_{\Gamma(0)} y_0(s) \partial_s x_0(s) \, ds, \quad t \geq 0, \]  \hspace{1cm} (2.6.25)

and the total energy of the thin film is decreasing during the evolution, i.e.,

\[ W_{\text{reg}}^\delta(t) \leq W_{\text{reg}}^\delta(t_1) \leq W_{\text{reg}}^\delta(0) = \int_{\Gamma(0)} (\gamma(\theta) + \delta^2 \kappa^2) \, ds - (x_c^r(0) - x_c^l(0)) \sigma, \quad t \geq t_1 \geq 0. \]  \hspace{1cm} (2.6.26)

**Proof.** The proof for the mass conservation is the same as that for the weak case. For the energy, based on the variation form in Eq. (2.6.15), we have:

\[
\frac{d}{dt} W_{\text{reg}}^\delta = - \int_{\Gamma} \left[ \partial_s \xi^\perp + \delta^2 (\kappa^3 + \partial_{ss} \kappa) \mathbf{n} \right] : \mathbf{X}_t \, ds \\
+ \frac{dx_c^r}{dt} [\xi_2 - \sigma - \delta^2 \partial_c \kappa n] \big|_{s=L} - \frac{dx_c^l}{dt} [\xi_2 - \sigma - \delta^2 \partial_c \kappa n] \big|_{s=0}. \]  \hspace{1cm} (2.6.27)

Using the Eq. (2.6.19), Eq. (2.6.20) and the contact line moving boundary conditions, we have:

\[
\frac{d}{dt} W_{\text{reg}}^\delta = \int_{\Gamma(0)} \mu \mu_{ss} \, ds - \frac{1}{\eta} \left[ \left( \frac{dx_c^l}{dt} \right)^2 + \left( \frac{dx_c^r}{dt} \right)^2 \right] \\
= - \int_{\Gamma(0)} (\mu_s)^2 \, ds - \frac{1}{\eta} \left[ \left( \frac{dx_c^l}{dt} \right)^2 + \left( \frac{dx_c^r}{dt} \right)^2 \right] \leq 0. \]  \hspace{1cm} (2.6.28)

Note the last identity follows from the zero mass flux boundary condition. \( \square \)
2.6 Extension to strongly anisotropic case

2.6.3 A discretization by PFEM

In order to obtain the variational formulation for equations (2.6.19), (2.6.20) with the boundary conditions (2.6.21)-(2.6.24), we need to introduce a new vector \( I \). Here we assume \( I \) is parallel to \( n \), thus we are able to rewrite the equations in the following form

\[
\partial_t X \cdot n = \partial_s \mu, \quad \mu \cdot n = -|\partial_s \xi|^\perp - \delta^2 I, \tag{2.6.29}
\]

\[
I \cdot n = \left( \frac{1}{2} \kappa^3 + \partial_s \kappa \right), \quad \kappa \cdot n = -\partial_s X. \tag{2.6.30}
\]

By using the integration by parts, the weak formulation for solid-state dewetting problems with strongly anisotropic surface energy can be stated as the following variational problem: given the initial curve \( \Gamma(0) = X(\rho, 0), \rho \in I \), for every time \( t \in (0, T) \), find the evolution curves \( \Gamma(t) = X(\rho, t) \in H^1_{a,b}(I) \times H^1_0(I) \) with the \( x \)-coordinate positions of moving contact points \( a = x_c^l(t) \leq x_c^r(t) = b \), the chemical potential \( \mu(\rho, t) \in H^1(I) \), \( I(\rho, t) \in H^1(I) \times H^1(I) \) and the curvature \( \kappa(\rho, t) \in H^1_0(I) \) such that

\[
\langle \partial_t X, \varphi \rangle_{\Gamma} + \langle \partial_s \mu, \partial_s \varphi \rangle_{\Gamma} = 0, \quad \forall \varphi \in H^1(I), \tag{2.6.31a}
\]

\[
\langle \mu, \omega_1 \rangle_{\Gamma} - \langle \xi^\perp, \partial_s \omega_1 \rangle_{\Gamma} - \delta^2 \langle I, \omega_1 \rangle_{\Gamma} + \langle \xi^\perp \cdot \omega_1 \rangle_{\Gamma}^{s=L(t)} = 0, \quad \forall \omega_1 \in (H^1(I))^2, \tag{2.6.31b}
\]

\[
\langle I, n \phi \rangle_{\Gamma} - \frac{1}{2} \langle \kappa^3, \phi \rangle_{\Gamma} + \langle \partial_s \kappa, \partial_s \phi \rangle_{\Gamma} = 0, \quad \forall \phi \in H^1_0(I), \tag{2.6.31c}
\]

\[
\langle \kappa n, \omega_2 \rangle_{\Gamma} - \langle \partial_t X, \partial_s \omega_2 \rangle_{\Gamma} = 0, \quad \forall \omega_2 \in (H^1_0(I))^2. \tag{2.6.31d}
\]

After temporal and spatial discretization, the full-discrete finite element scheme for the variational formulation (2.6.31a)-(2.6.31d) then can be described as: given the curve \( \Gamma^m = X^m \) \( (m = 0, 1, \ldots, M - 1) \), for the next time level \( t_{m+1} \), find the numerical solution for evolution curves \( \Gamma^{m+1} = X^{m+1} \in V^h_{a,b} \times V^h_0 \) with the \( x \)-coordinate positions of moving contact points \( a = x_c^l(t_{m+1}) \leq x_c^r(t_{m+1}) = b \), the numerical solution for \( \Gamma^{m+1} \in V^h \times V^h \), chemical potential \( \mu^{m+1} \in V^h \) and the
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numerical solution for curvature $\kappa^{m+1} \in V_0^h$ such that:

$$\frac{X^{m+1} - X^m}{\tau_m}, \varphi_h \mathbf{n}^m \big|_{\Gamma_m^h} + (\partial_s \mu^{m+1}, \partial_s \varphi_h)^h_{\Gamma_m} = 0, \quad \forall \varphi_h \in V^h, \tag{2.6.32a}$$

$$\left(\mu^{m+1} \mathbf{n}^m - \delta^2 \mathbf{I}^{m+1}, \omega_1^h\right)^h_{\Gamma_m} - \left(\left(\kappa^m\right)^\perp, \partial_s \omega_1^h\right)^h_{\Gamma_m} = -\left(\left(\kappa^m\right)^\perp \cdot \omega_1^h\right)^h_{\rho=1}, \quad \forall \omega_1^h \in (V^h)^2, \tag{2.6.32b}$$

$$\left(\mathbf{I}^{m+1}, \mathbf{n}^m \phi_h\right)^h_{\Gamma_m} - \frac{1}{2} \left(\left(\kappa^m\right)^2 \kappa^{m+1}, \phi_h\right)^h_{\Gamma_m} + (\partial_s \kappa^{m+1}, \partial_s \phi_h)^h_{\Gamma_m} = 0, \quad \forall \phi_h \in V_0^h, \tag{2.6.32c}$$

$$\left(\kappa^{m+1} \mathbf{n}^m, \omega_2^h\right)^h_{\Gamma_m} - (\partial_s X^m, \partial_s \omega_2^h)^h_{\Gamma_m} = 0, \quad \forall \omega_2^h \in (V_0^h)^2. \tag{2.6.32d}$$

Here $x_c^l(t_{m+1})$ and $x_c^r(t_{m+1})$ are updated from Eqs. (2.6.22) by Euler forward scheme.

2.6.4 Numerical results

In the following, we will present some numerical convergence tests of our fully discrete scheme (2.6.32a),(2.6.32b),(2.6.32c),(2.6.32d). Similar to the weak anisotropy, we perform our numerical scheme on both closed curve evolution and open curve evolution (solid-state dewetting). For closed curve evolution, shown in Table. 2.5, the initial shape of thin film is chosen as a closed tube, i.e., a rectangle of length 4 and width 1 added by two semi-circles with radii of 0.5 to its left and right sides, and the parameters are chosen as $h_0 = (8 + \pi)/120$ and $\tau_0 = 0.005$; for an open curve evolution, shown in Table 2.4, the initial shape of thin film is chosen as a rectangle island of length 5 and thickness 1, and $h_0 = 0.1$ and $\tau_0 = 0.0005 = 0.05h_0^2$. Table. 2.5 shows the convergence rate in the $L^\infty$ norm for a closed curve evolution under the strongly anisotropic surface diffusion flow, where $\gamma(\theta) = 1 + 0.1 \cos(4\theta), \delta = 0.1$. It clearly shows that the convergence order is around second order, while for open curves, the convergence order decrease to first order. Same as the isotropic/weakly anisotropic case, the decrease of the convergence order may due to the application of the forward Euler scheme on the relaxed contact angle conditions.

Fig. 2.17 plots the numerical equilibrium shapes for $\delta = 0.2, 0.1, 0.05$ as well as the theoretical equilibrium shape (show in solid blue line) under the parameter $\sigma =$
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Table 2.5: Convergence rates in the $L^\infty$ norm for a closed curve evolution under the anisotropic surface diffusion flow, where $\gamma(\theta) = 1 + 0.1 \cos(4\theta), \delta = 0.1$.

<table>
<thead>
<tr>
<th>$e_{h,\tau}(t)$</th>
<th>$h = h_0$</th>
<th>$h_0/2$</th>
<th>$h_0/2^2$</th>
<th>$h_0/2^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e_{h,\tau}(t = 0.5)$</td>
<td>1.54E-3</td>
<td>6.22E-4</td>
<td>1.57E-4</td>
<td>3.80E-5</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>1.31</td>
<td>1.98</td>
<td>2.07</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 2.0)$</td>
<td>7.66E-4</td>
<td>2.21E-4</td>
<td>5.51E-4</td>
<td>1.30E-5</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>1.79</td>
<td>2.01</td>
<td>2.06</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 5.0)$</td>
<td>7.52E-4</td>
<td>2.10E-4</td>
<td>5.32E-4</td>
<td>1.30E-5</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>1.84</td>
<td>1.98</td>
<td>2.03</td>
</tr>
</tbody>
</table>

Table 2.6: Convergence rates in the $L^\infty$ norm for an open curve evolution under the strongly anisotropic surface diffusion flow (solid-state dewetting with isotropic surface energy), where $\gamma(\theta) = 1 + 0.1 \cos(4\theta), \delta = 0.1, \sigma = \cos(5\pi/6)$.

<table>
<thead>
<tr>
<th>$e_{h,\tau}(t)$</th>
<th>$h = h_0$</th>
<th>$h_0/2$</th>
<th>$h_0/2^2$</th>
<th>$h_0/2^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e_{h,\tau}(t = 0.5)$</td>
<td>3.25E-2</td>
<td>1.60E-2</td>
<td>8.14E-3</td>
<td>4.16E-3</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>1.02</td>
<td>0.98</td>
<td>0.97</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 2.0)$</td>
<td>2.67E-2</td>
<td>1.41E-2</td>
<td>7.23E-3</td>
<td>3.70E-3</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>0.92</td>
<td>0.97</td>
<td>0.97</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 5.0)$</td>
<td>2.33E-2</td>
<td>1.18E-3</td>
<td>6.02E-3</td>
<td>3.05E-3</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>0.98</td>
<td>0.98</td>
<td>0.98</td>
</tr>
</tbody>
</table>
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Figure 2.17: Comparison of the numerical equilibrium shapes of thin island film with its theoretical equilibrium shape for several values of regularization parameter $\delta$, where the solid black lines represent the theoretical equilibrium and colored lines represent the numerical equilibriums, and $\gamma(\theta) = 1 + 0.2 \cos(4\theta), \sigma = \cos(2\pi/3)$. The numerical equilibrium shapes converge to the theoretical equilibrium shape when the regularization parameter $\epsilon$ approaches zero.

The numerical equilibrium shapes converge to the theoretical equilibrium shape when the regularization parameter $\epsilon$ approaches zero.

Fig. 2.18 shows the numerical equilibrium shapes for several different anisotropies with different anisotropy strength $\beta$ and $k$-fold crystalline symmetries under the fixed parameters $\phi = 0, \sigma = \cos(3\pi/4), \delta = 0.1$. Fig. 2.18(a) and Fig. 2.18(b) shows the effects of increasing the anisotropy strength from $\beta = 0.1$ to $\beta = 0.3$ with fixed $k = 4$. We can observe that the equilibrium shape becomes almost perfectly "faceting". The effect of rotational symmetry representing by the parameter $k$ can be observed in Fig. 2.18(c) ($k = 3, \beta = 0.3$) and Fig. 2.18(d) ($k = 6, \beta = 0.1$).

Fig. 2.19 shows the dynamic evolution of the initial rectangle (show in solid red line) towards its equilibrium shape (solid blue line) for $\delta = 0.1$ at several time steps. We can observe that wavy structure (Fig. 2.19(b)) appears during the evolution.

The corresponding temporal evolution of the free energy and area are shown in
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Figure 2.18: Equilibrium island morphologies for a small, initially rectangular island under several different crystalline fold of symmetry $k$ and degree of anisotropy $\beta$ respectively. (a) $k = 4, \beta = 0.1$; (b) $k = 4, \beta = 0.3$; (c) $k = 3, \beta = 0.3$; (d) $k = 6, \beta = 0.1$. The other computational parameters are chosen as, $\phi = 0, \sigma = \cos(3\pi/4), \delta = 0.1$.

Figure 2.19: The evolution of a small initial island (red line) to the equilibrium (blue line), where $\gamma(\theta) = 1 + 0.2\cos(4\theta), \sigma = \cos(2\pi/3), \delta = 0.1$. (a) $t = 0$; (b) $t = 0.02$; (c) $t = 0.04$; (d) $t = 10.32$. 
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Figure 2.20: (a) The temporal evolution of the normalized free energy and normalized area, (b) the temporal evolution of the mesh distribution function $\psi(t)$, where $\gamma(\theta) = 1 + 0.2 \cos(4\theta)$, $\sigma = \cos \frac{2\pi}{3}$, $\delta = 0.1$.

Fig. 2.20. From the figure, we can observe that the area conservation and energy dissipation are well satisfied for the discrete numerical solutions. Moreover, Fig. 2.20(b) shows the value of mesh distribution function during the evolution. The mesh distribution function is cut from the top at value 20 because of the artificial re-mesh during the evolution when $\psi$ is bigger than 20. We find that when the surface energy is strongly anisotropic, the mesh could be deteriorated in a very short time from the initial. Thus this re-mesh is essential and necessary to enable the stability of the scheme. Luckily, it is only needed in the earlier stage of the evolution and the mesh can be well preserved in the later time.
Chapter 3

A Sharp Interface Model in Three Dimensions

Figure 3.1: A schematic illustration of solid-state dewetting on a rigid flat substrate in three dimensions.

As depicted in Figure 3.1, a solid thin film (colored in blue) lies on a flat rigid
substrate (colored in gray). The moving film/vapor interface is geometrically described by a two-dimensional open manifold $S$ with boundary $\Gamma$, where $\Gamma$ is a closed plane curve attached to the flat substrate $S_{\text{sub}}$. The unit vector $\mathbf{n}$ represents the normal direction of $S$ and points towards the vapour while $\mathbf{n}_{\Gamma}$, $\mathbf{\tau}_{\Gamma}$ and $\mathbf{c}_{\Gamma}$ are three unit vectors defined along the boundary $\Gamma$. Exactly, $\mathbf{n}_{\Gamma}$ is the outer unit normal vector of the plane curve $\Gamma$ on the substrate $S_{\text{sub}}$. $\mathbf{\tau}_{\Gamma}$ is the unit tangent vector of $\Gamma$ on the substrate $S_{\text{sub}}$ and pointing in the counter-clockwise direction when viewed from the $+z$ axis. The unit vector $\mathbf{c}_{\Gamma}$, called the co-normal vector, is normal to $\Gamma$, tangent to $S$ and pointing outwards, see Fig. 3.1. In other words, for $\mathbf{x} \in S$, if we denote $\mathcal{T}_x S$ and $\mathcal{N}_x S$ as the tangent and normal space to $S$ respectively, then the following expressions hold,

$$
\mathbf{n}(\mathbf{x}) \in \mathcal{N}_x S, \quad \forall \mathbf{x} \in S,
$$

$$
\mathbf{c}_{\Gamma}(\mathbf{x}) \in \mathcal{T}_x S, \quad \mathbf{c}_{\Gamma}(\mathbf{x}) \perp \mathbf{\tau}_{\Gamma}, \quad \forall \mathbf{x} \in \Gamma,
$$

$$
\mathbf{n}_{\Gamma}(\mathbf{x}) \perp \mathbf{\tau}_{\Gamma}, \quad \mathbf{n}_{\Gamma}(\mathbf{x}) \parallel S_{\text{sub}}, \quad \forall \mathbf{x} \in \Gamma.
$$

(3.0.1)

Now from Eq. (1.2.3), the total surface energy of the system can be written as

$$
W = W_{\text{int}} + W_{\text{sub}} = \int_S \gamma(\mathbf{n}) \, dS + (\gamma_{FS} - \gamma_{VS}) A(\Gamma).
$$

(3.0.2)

Here in these expressions, $\gamma_{FV}$, $\gamma_{FS}$ and $\gamma_{VS}$ represent the energy densities of the film/vapor, film/substrate and vapor/substrate respectively. $A(\Gamma)$ denotes the area enclosed by the the plane curve $\Gamma$ on the substrate. We assume that $\gamma_{FS}$ and $\gamma_{VS}$ are constants, while $\gamma_{FV} = \gamma(\mathbf{n})$ is dependent on the orientation of the film/vapor interface. The total surface energy is composed of two parts, the interfacial energy of film/vapor interface denoted by $W_{\text{int}}$, and the substrate energy denoted by $W_{\text{sub}}$.

The derivation of the three-dimensional sharp interface model seems quite straightforward by simply repeating the procedure in chapter 2 as long as we are given the energy equation. However, performing the thermodynamic variation of the surface integral $W_{\text{int}}$ is not as easy as we think. In short, there are two major difficulties in calculating the first variation. Firstly, if $S$ is a closed surface, then the perturbation of the surface in the tangential direction would contribute nothing to the first
variation. Thus only the perturbation in the normal direction will be considered and the variation of some geometric objects such as the normal vector, the mean curvature can be directly obtained [34]. However, when it comes to the solid-state dewetting problem, the infinitesimal perturbation of the surface in the tangential direction could be essential to the first variation of the surface energy. More precisely, the interface $S$ is open and the tangent deformation on the boundary of $S$ plays an important role in investigating the contact line migration along the substrate [9, 67]. Secondly, unlike 2D, calculating the variation via the parameterization of the surface could be too tedious to perform in three dimensions. Therefore in this chapter, we are engaged in the derivation of the three-dimensional sharp interface model. We will develop the sharp interface model rigorously with the help of speed method and shape derivatives from shape sensitivity analysis [109]. This approach avoids the parameterization of the surface on a fixed reference domain and is able to deal with perturbation in arbitrary direction [39, 64, 109].

3.1 Shape differential calculus

We start by introducing some basic knowledge about surface calculus and differential geometry. For more related knowledge, please refer to the [45, 109].

3.1.1 Hypersurface

Definition 3.1.1 (C$^k$-hypersurface). $S \subset \mathbb{R}^3$ is called a $C^k$-hypersurface, where $k \in \mathbb{N} \cup \{\infty\}$, if for each point $x_0 \in S$, there exists an open set $U \subset \mathbb{R}^3$ containing $x_0$ and a function $\phi \in C^k(U)$, such that

$$U \cap S = \{x \in U \mid \phi(x) = 0\}, \quad \nabla \phi(x) \neq 0, \ \forall x \in U \cap S. \quad (3.1.1)$$

In view of the definition of hypersurface, we know that the normal vector of $S$ at point $x$ can be locally computed as $\frac{\nabla \phi(x)}{|\nabla \phi(x)|}$ or $-\frac{\nabla \phi(x)}{|\nabla \phi(x)|}$. 
Definition 3.1.2. A function \( f \in C^2(S) \) is defined on a \( C^2 \)-hypersurface \( S \subset \mathbb{R}^3 \). If \( n \) is the unit normal vector of \( S \), and \( \bar{f} \) is an arbitrary extension of \( f \) in the neighbourhood of \( S \) in \( \mathbb{R}^3 \), the surface gradient of \( f \) on \( S \) is defined as

\[
\nabla_S f = \nabla \bar{f} - (\nabla \bar{f} \cdot n) n.
\]

(3.1.2)

It is easy to prove that \( \nabla_S f \) is independent of the extension of \( f \) and only reliable on the value of \( f \) on \( S \). We can write \( \nabla_S \) as a vector operator

\[
\nabla_S = (D_1, D_2, D_3),
\]

(3.1.3)

then the surface divergence of function \( \mathbf{g} = (g_1, g_2, g_3) \in [C^1(S)]^3 \) is given by

\[
\nabla_S \cdot \mathbf{g} = \sum_{i=1}^{3} D_i g_i.
\]

(3.1.4)

Moreover, the Laplace-Beltrami operator can be expressed as

\[
\Delta_S f = \nabla_S \cdot \nabla_S f = \sum_{i=1}^{3} D_i^2 f.
\]

(3.1.5)

Here \( \nabla_S f \) comes from the gradient of \( \bar{f} \) by subtracting the normal components. Thus we know that \( \nabla_S f(x) \in T_x S, \forall x \in S \). We can also define the following matrix \( H \) such that the its element is taken as

\[
H_{ij} = D_i n_j.
\]

(3.1.6)

This matrix is called the extended Weingarten map with a zero eigenvalue in normal direction and two other eigenvalues given by the two principle curvatures of \( S \). The mean curvature is the trace of the matrix

\[
\mathcal{H} = \sum_{i=1}^{3} H_{ii} = \nabla_S \cdot n.
\]

(3.1.7)

If we denote \( \kappa_1 \) and \( \kappa_2 \) as the two principle curvatures, by noting the eigenvalues of \( H \), we have that

\[
\text{trace}(H^2) = \kappa_1^2 + \kappa_2^2 = \mathcal{H}^2 - 2\mathcal{K},
\]

(3.1.8)

with \( \mathcal{K} \) representing the Gaussian curvature.

The formula for integration by parts on surface \( S \) reads as
Theorem 3.1.1 ([45], p.297, Thm. 2.10). Assume $S$ is a hypersurface in $\mathbb{R}^3$ with smooth boundary $\Gamma$, $f \in H^1(S)$, then we have

$$\iint_S \nabla_S f \, dS = \iint_S f \mathcal{H} n \, dS + \int_{\Gamma} f c_r \, d\Gamma,$$

(3.1.9)

where $n$ and $c_r$ are the normal vector and co-normal vector respectively. $\mathcal{H}$ is the mean curvature.

The following proposition can be directly obtained from above theorem.

Proposition 3.1.1. Let $S$ be a hypersurface in $\mathbb{R}^3$ with smooth boundary $\Gamma$, and $f$ and $g$ belong to $H^1(S)$, we have

$$\iint_S \nabla_S fg \, dS = -\iint_S f \nabla_S g \, dS + \iint_S fg \mathcal{H} n \, dS + \int_{\Gamma} fg c_r \, d\Gamma,$$

(3.1.10)

by using the fact that $\nabla_S (fg) = \nabla_S f g + f \nabla_S g$.

3.1.2 Parameterized hypersurface

Definition 3.1.3 (Parametrized $C^k$-surface). We call $S \in \mathbb{R}^3$ is a parameterized $C^k$-surface, where $k \in \mathbb{N} \cup \infty$, if for every $x \in S$, there exists an open set $V \in \mathbb{R}^3$ with $x \in V$, an open connected set $U \in \mathbb{R}^2$ and a map $X : U \to V \cap S$ such that $X \in C^k(U, \mathbb{R}^3)$ and $X$ is bijective with rank($\nabla X$) = 2 on $U$. Then the map $X$ is called a local parameterization of $S$.

We have the following lemma for the relationship between the parameterized surface and hypersurface.

Lemma 3.1.1 (Lemma 2.2 in [45]). Assume $S$ is a $C^k$-hypersurface in $\mathbb{R}^3$. Then for every $x \in S$, there exist an open set $V \in \mathbb{R}^3$ with $x \in V$ and a parameterized $C^k$-surface $X : U \to V \cap S$ such that $X$ is a bijective map from $U$ to $V \cap S$. On the other hand, if $X : U \to V \cap S$ is a parameterized $C^k$-surface, then there is an open set $\hat{U} \subset U$ such that $X(\hat{U})$ is a $C^k$-hypersurface.
Let $X \in C^4(U, \mathbb{R}^3)$ be a local parametrization of $S$, and $(u_1, u_2) \in U$, the first fundamental form can be given by

$$G(u, v) = (g_{ij})_{i,j=1,2}, \text{ with } g_{ij} = \frac{\partial X}{\partial u_i} \cdot \frac{\partial X}{\partial u_j}. \tag{3.1.11}$$

Let $g = \det(G)$. Besides, the inversion of matrix $G$ is denote by

$$G^{-1} = (g^{ij})_{i,j=1,2}. \tag{3.1.12}$$

Now given a function $f : S \to \mathbb{R}$ defined $S$, let $F(u_1, u_2) = f(X(u_1, u_2))$, the surface gradient of $f$ can be expressed in terms of the parameters as

$$\nabla_S f = \sum_{i,j=1}^{2} g^{ij} \frac{\partial F}{\partial u_i} \cdot \frac{\partial X}{\partial u_j}. \tag{3.1.13}$$

Moreover, we have

$$\Delta_S f = \frac{1}{g} \sum_{i,j=1}^{2} \frac{\partial}{\partial u_j} (g^{ij} \sqrt{g} \frac{\partial F}{\partial u_i}). \tag{3.1.14}$$

### 3.1.3 Shape derivatives

To carry out the first variation of the integral on a manifold, we need to introduce a family of perturbations. Consider a domain $D \in \mathbb{R}^3$ with the boundary $\partial D$ which is piecewise $C^k$ for a given integer $k \geq 0$, we can define the transformation as

$$T_\varepsilon : \bar{D} \to \bar{D}, \quad \varepsilon \in [0, \varepsilon_0), \tag{3.1.15}$$

where $T_\varepsilon$ is a one-to-one map. Here we assume that $T_\varepsilon$ and $T_\varepsilon^{-1}$ belong to $C^k(\bar{D}, \bar{D})$ for all $\varepsilon \in [0, \varepsilon_0)$, also $T_\varepsilon$ belongs to $C^k([0, \varepsilon_0))$ for all $x \in \bar{D}$, where $k \in \mathbb{N} \cup \{\infty\}$. Now under this transformation, a bounded domain $\Omega$ or surface $S$ in $\bar{D}$ will be changed to

$$\Omega_\varepsilon = T_\varepsilon(\Omega), \quad S_\varepsilon = T_\varepsilon(S), \tag{3.1.16}$$

with $S_0 = S, \Omega_0 = \Omega$.

Let $x(X, \varepsilon) = T_\varepsilon(x)$, the speed vector field $V(x, \varepsilon)$ at point $x$ is defined as

$$V(x, \varepsilon) = \frac{\partial x}{\partial \varepsilon} (T_\varepsilon^{-1}(x), \varepsilon). \tag{3.1.17}$$
Now we consider the following ODEs:

\[
\frac{d}{d\varepsilon} x(X, \varepsilon) = V(x(X, \varepsilon), \varepsilon),
\]

\[
x(X, 0) = X,
\]  

(3.1.18)

with \( X \in D \). The existence of the one-to-one map has been shown by Theorem 2.16 in [109]. In other words, as long as the vector field \( V \) satisfy \( V \in C(C^k(D, \bar{D}); [0, \varepsilon_0]) \), then it uniquely determines the transformations \( T_\varepsilon \). Thus the transformation \( T_\varepsilon \) and the \( V \) are uniquely determined by each other. In the following, when the vector field \( V \) is introduced, we use \( T_\varepsilon(V) \) to denote the corresponding transformation. For simplicity, we also assume \( V_0 = V(X, 0) \).

We have the following lemma for the transformation \( T_\varepsilon(V) \).

**Lemma 3.1.2** (Lemma. 2.44, Lemma 2.49 in [109]). Assume \( D \in \mathbb{R}^3 \) is a bounded domain, and \( V \in C(C^k(\bar{D}, \bar{D}); [0, \varepsilon_0]) \) is the given vector field with \( k \geq 1 \), such that \( V \cdot n = 0 \) a.e on \( \partial D \). Furthermore, it is assumed that \( V = 0 \) at any singular point of \( \partial D \). If \( DT_\varepsilon \) is the Jacobian matrix of the transformation \( T_\varepsilon \), that is

\[
DT_\varepsilon = \left( \frac{\partial T_\varepsilon i(V)}{\partial X_j}(X) \right)_{i,j=1,2,3}.
\]  

(3.1.19)

Define \( \zeta(x, \varepsilon) \) and \( \omega(x, \varepsilon) \) as follows

\[
\zeta(X, \varepsilon) = \det(DT_\varepsilon),
\]  

(3.1.20a)

\[
\omega(X, \varepsilon) = \zeta(X, \varepsilon)||DT_\varepsilon^{-T} n||,
\]  

(3.1.20b)

then we have

\[
\frac{\partial \zeta(X, \varepsilon)}{\partial \varepsilon} \bigg|_{\varepsilon=0} = \nabla \cdot V_0,
\]  

(3.1.21a)

\[
\frac{\partial \omega(X, \varepsilon)}{\partial \varepsilon} \bigg|_{\varepsilon=0} = \nabla_s \cdot V_0.
\]  

(3.1.21b)

Functions \( \zeta(X, \varepsilon) \) and \( \omega(X, \varepsilon) \) will be useful in performing the change of variables of the domain and surface integrals.

We can define the first variation of the shape functionals as follows.
Definition 3.1.4 (First variation). Let $J(\Omega)$ be a shape functional, and $\Omega$ is a bounded domain in $\bar{D}$, the first variation of the functional $J(\Omega)$ at $\Omega$ in the direction of the vector field $V \in C(C^k(\bar{D}, \bar{D}); [0, \varepsilon_0])$ is given as a limit:

$$dJ(\Omega; V) = \lim_{\varepsilon \to 0} \frac{J(\Omega_{\varepsilon}) - J(\Omega)}{\varepsilon}. \quad (3.1.22)$$

Similarly, let $J(S)$ be a shape functional, the first variation of the functional $J(S)$ at $S$ in the direction of the vector field $V$ is given as a limit:

$$dJ(S; V) = \lim_{\varepsilon \to 0} \frac{J(S_{\varepsilon}) - J(S)}{\varepsilon}. \quad (3.1.23)$$

Definition 3.1.5 (Material derivative, [109], Def.2.71, Def.2.74). The material derivative $\dot{\varphi}(\Omega; V)$ of $\varphi$ on $\Omega$ in the direction $V$ is given as

$$\dot{\varphi}(\Omega; V) = \lim_{\varepsilon \to 0} \frac{\varphi(\Omega_{\varepsilon}) \circ T_\varepsilon(V) - \varphi}{\varepsilon}. \quad (3.1.24)$$

Similarly, the material derivative $\dot{\varphi}(S; V)$ of $\varphi$ on $S$ in the direction $V$ is given as

$$\dot{\varphi}(S; V) = \lim_{\varepsilon \to 0} \frac{\varphi(S_{\varepsilon}) \circ T_\varepsilon(V) - \varphi}{\varepsilon}. \quad (3.1.25)$$

The above material derivative is the derivative with respect to the moving coordinate systems. On the other hand, we can define the shape derivative of $\varphi$ in the following by subtracting the term $(\nabla \varphi) \cdot V_0$, which represents the derivative with respect to the stationary coordinates.

Definition 3.1.6. [Shape derivative on domain, [109], Def.2.85] The shape derivative $\varphi'(\Omega; V)$ of $\varphi$ on $\Omega$ in the direction $V$ is given as

$$\varphi'(\Omega; V) = \varphi(\Omega; V) - \nabla \varphi(\Omega) \cdot V_0. \quad (3.1.26)$$

As can be seen, if $\varphi$ is independent of $\Omega$, we can obtain $\varphi'(\Omega; V) = 0$. We have the following lemma for the first variation of the domain integrals.

Lemma 3.1.3. Let $\Omega$ be a domain in $\bar{D}$ and its boundary $\partial \Omega$ is smooth enough, $y(\Omega) \in L^1(\Omega)$ is a function such that the material derivative $\dot{y}(\Omega; V)$ exists or exists in the weak sense and $\dot{y}(\Omega; V) \in L^1(\Omega)$, let $J(\Omega) = \iint_\Omega y(\Omega) \, dx$, then we have

$$dJ(\Omega; V) = \iiint_\Omega \dot{y}(\Omega; V) \, dX + \iiint_\Omega y(\Omega) \nabla \cdot V_0 \, dX. \quad (3.1.27)$$
Furthermore, if the shape derivative $y'(\Omega; V)$ exists and $\nabla y(\Omega) \cdot V_0 \in L^1(\Omega)$, we then have

$$dJ(\Omega; V) = \iiint_{\Omega} y'(\Omega; V) \, dX + \int_{\partial \Omega} y(\Omega) V_0 \cdot n \, dS,$$

(3.1.28)

where we use $dX, dx$ as integration on domain $\Omega, \Omega_\varepsilon$, respectively.

**Proof.** For the shape functional $J(\Omega_\varepsilon) = \iiint_{\Omega_\varepsilon} y(\Omega_\varepsilon) \, dx$, using the change of variables $x = T_\varepsilon(V)(X)$ for $J(\Omega_\varepsilon)$, we have

$$J(\Omega_\varepsilon) = \iiint_{\Omega} y(\Omega_\varepsilon) \circ T_\varepsilon(V) \zeta(X, \varepsilon) \, dX.$$ \hspace{1cm} (3.1.29)

By noting the fact that $\zeta(X, 0) = 1$, we obtain the following equations,

$$dJ(\Omega; V) = \lim_{\varepsilon \to 0} \frac{J(\Omega_\varepsilon) - J(\Omega)}{\varepsilon} = \iiint_{\Omega} \left[ \lim_{\varepsilon \to 0} \frac{y(\Omega_\varepsilon) \circ T_\varepsilon(V) \zeta(X, \varepsilon) - y(\Omega) \circ T_0(V) \zeta(X, 0)}{\varepsilon} \right] dX = \iiint_{\Omega} \left[ \dot{y}(\Omega; V) \zeta(X, 0) + y(\Omega) \frac{\partial \zeta(X, \varepsilon)}{\partial \varepsilon} \Big|_{\varepsilon=0} \right] dX.$$ \hspace{1cm} (3.1.30)

In view of lemma. 3.1.2, the above equations can be changed to

$$dJ(\Omega; V) = \iiint_{\Omega} \dot{y}(\Omega; V) \, dX + \iiint_{\Omega} y(\Omega) \nabla \cdot V_0 \, dX.$$ \hspace{1cm} (3.1.31)

Using the equation $y(\Omega) \nabla \cdot V_0 + (\nabla y(\Omega)) \cdot V_0 = \nabla \cdot (y(\Omega) V_0)$, we obtain

$$dJ(\Omega; V) = \iiint_{\Omega} [\dot{y}(\Omega; V) - \nabla y(\Omega) \cdot V_0] \, dX + \iiint_{\Omega} \nabla \cdot (y(\Omega) V_0) \, dX. \hspace{1cm} (3.1.32)$$

Now by the definition of shape derivative on the domain $\Omega$ (Definition. 3.1.6), and also applying stokes formula for the second term, we finally get

$$dJ(\Omega; V) = \iiint_{\Omega} y'(\Omega; V) \, dX + \int_{\partial \Omega} y(\Omega) V_0 \cdot n \, dS,$$

(3.1.33)

Different to the shape derivative on the domain, the shape derivative on the surface is defined in the following,
3.1 Shape differential calculus

Definition 3.1.7. [Shape derivative, [109], Def.2.88] The shape derivative $\psi'(S; V)$ of $\psi$ on $S$ in the direction $V$ is given as

$$
\psi'(S; V) = \dot{\psi}(S; V) - \nabla_s \psi(S) \cdot V_0. \tag{3.1.34}
$$

Now let us consider the shape functional $J(S_\varepsilon) = \int_S \varphi(S_\varepsilon) \, dS_\varepsilon$, we have the following lemma.

Lemma 3.1.4. Let $S$ be a two-dimensional manifold in $\bar{D}$ with smooth boundary $\Gamma$, $\varphi(S) \in L^1(S)$ is a function such that the material derivative $\dot{\varphi}(S; V)$ exists or exists in the weak sense and $\varphi(S; V) \in L^1(S)$, let $J(S) = \int_S \varphi(S) \, dS$, then we have

$$
dJ(S; V) = \int_S \dot{\varphi}(S; V) \, dS + \int_S \varphi(S) \nabla_s \cdot V_0 \, dS. \tag{3.1.35}
$$

Furthermore, if the shape derivative $\varphi'(S; V)$ exists and $\nabla_s \varphi \cdot V_0 \in L^1(S)$, we have

$$
dJ(S; V) = \int_S \varphi'(S; V) \, dS + \int_S \varphi(S) \nabla_s \cdot V_0 \, dS + \int_\Gamma \varphi(S) V_0 \cdot c_\Gamma \, d\Gamma. \tag{3.1.36}
$$

Proof. For the shape functional $J(S)$ under the variation vector field $V$, we have

$$
J(S_\varepsilon) = \int_S (\varphi \circ T_\varepsilon(V)) \omega(X, \varepsilon) \, dS, \tag{3.1.37}
$$

where $\omega(X, \varepsilon)$ is defined in Lemma. 3.1.2. By using the fact that $\omega(X, 0) = 1$ and Lemma. 3.1.2, we obtain the following equations

$$
dJ(S; V) = \lim_{\varepsilon \to 0} \frac{J(S_\varepsilon) - J(S)}{\varepsilon}
= \int_S \lim_{\varepsilon \to 0} \frac{[\varphi(S_\varepsilon) \circ T_\varepsilon(V) \omega(X, \varepsilon) - \varphi \circ T_0(V) \omega(X, 0)]}{\varepsilon} \, dS
= \int_S \dot{\varphi}(S; V) \omega(X, 0) \, dS + \int_S \varphi(S) \frac{\partial \omega(X, \varepsilon)}{\partial \varepsilon} \bigg|_{\varepsilon=0} \, dS
= \int_S \dot{\varphi}(S; V) \, dS + \int_S \varphi(S) \nabla_s \cdot V_0 \, dS. \tag{3.1.38}
$$

For the second term, using Eq. (3.1.10) and integration by parts, also noting the
definition of the shape derivative on $S$, we obtain directly

$$
\frac{dJ}{ds}(S; V) = \int_S \varphi'(S; V) dS - \int_S \nabla \varphi(S) \cdot V_0 dS + \int_S \varphi(S) V'_0 \cdot n_H dS
+ \int_{\Gamma} \varphi(S) V'_0 \cdot c_r d\Gamma
= \int_S \varphi'(S; V) dS + \int_S \varphi(S) H V'_0 \cdot n dS
+ \int_{\Gamma} \varphi(S) V'_0 \cdot c_r d\Gamma.
$$

(3.1.39)

Moreover, we have the following theorem based on above lemma.

**Theorem 3.1.2.** Assume $S \in \tilde{\mathcal{D}}$ is a two dimensional manifold with smooth boundary $\Gamma$, let $J(S) = \int_S \varphi(S) dS$ with $\varphi(S) \in H^1(S)$, $V$ is the variation vector field such that $V \in C(C^k(\tilde{D}; \tilde{D}); [0, \varepsilon_0])$, if the shape derivative $\varphi'(S; V)$ exist and $\varphi'(S; V) \in L^1(S)$, then we have

$$
\frac{dJ}{ds}(S; V) = \int_S \varphi'(S; V) dS + \int_S \varphi(S) H V'_0 \cdot n dS + \int_{\Gamma} \varphi(S) V'_0 \cdot c_r d\Gamma.
$$

(3.1.40)

Furthermore, if $y(\Omega)$ is a function defined on $\Omega$ such that $y(\Omega)|_S = \varphi(S)$, we have

$$
\frac{dJ}{ds}(S; V) = \int_S y'(Ω, V)|_S dS + \int_S \left[ \partial n y + y H \right] V'_0 \cdot n dS + \int_{\Gamma} y V'_0 \cdot c_r d\Gamma.
$$

(3.1.41)

**Proof.** The proof of this theorem is straightforward by noting the definition of shape derivatives on $\Omega$ and $S$ with above lemma.

Given a arbitrary function defined on $S$, the shape derivative is not easy to calculate. Luckily, with the help of the signed distance function, the shape derivative of the normal vector and the mean curvature can be obtained. Consider a closed domain $\Omega \in \mathbb{R}^3$ with its smooth boundary $\partial \Omega$, the signed distance function is given as

$$
b(x) = \begin{cases}
\text{dist}(x, \partial \Omega), & \forall x \in \mathbb{R}^3 / \Omega, \\
0, & \forall x \in \partial \Omega, \\
-\text{dist}(x, \partial \Omega), & \forall x \in \Omega.
\end{cases}
$$

(3.1.42)
Here \( \text{dist}(\mathbf{x}, \partial \Omega) = \inf_{y \in \partial \Omega} ||\mathbf{x} - \mathbf{y}|| \). The signed distance function has significant relationships with the normal vector and mean curvature of the surface \( \partial \Omega \). Precisely, we can extend the normal vector \( \mathbf{n} \) and mean curvature \( \mathcal{H} \) in a tubular neighbourhood in the following

\[
\mathbf{n}(\mathbf{x}) = \nabla b(\mathbf{x})\bigg|_{\partial \Omega}, \quad \mathcal{H}(\mathbf{x}) = \Delta b(\mathbf{x})\bigg|_{\partial \Omega}.
\] (3.1.43)

**Lemma 3.1.5** ([64]). Assume that \( \Omega \in \mathbb{R}^3 \) is a closed domain with smooth boundary \( \partial \Omega \), \( S \subset \partial \Omega \) is an open two-dimensional manifold, then the shape derivative of the unit normal vector \( \mathbf{n} \) and the mean curvature \( \mathcal{H} \) of \( S \) in the direction of velocity \( \mathbf{V} \) are given as

\[
\mathbf{n}' = \mathbf{n}'(\Omega; \mathbf{V})\bigg|_S = -\nabla_s (\mathbf{V}_0 \cdot \mathbf{n}), \quad \mathcal{H}' = \mathcal{H}'(\Omega; \mathbf{V})\bigg|_S = -\Delta_s (\mathbf{V}_0 \cdot \mathbf{n}).
\] (3.1.44)

### 3.2 Thermodynamic variation

In this section, we will calculate the thermodynamic variation of the surface energy defined in Eq. (3.0.2) for solid-state dewetting. Assume \( \Omega \) is a domain with smooth boundary in \( \mathbb{R}^3 \), the interface between the vapor and the film denote by \( S \) is contained in \( \Omega \), and the substrate denoted by \( S_{\text{sub}} \) is in the \( xOy \) plane. \( T_\varepsilon \) is a transformation of the domain \( \Omega \) such that \( T_\varepsilon \Gamma \subset S_{\text{sub}} \), which ensures that the contact line is always on the substrate.

Now for the first part of the surface energy \( W_{\text{int}} = \int_S \gamma(\mathbf{n}) dS \), assume \( \hat{\gamma} \) is the homogenous extension of \( \gamma(\mathbf{n}) \) from \( S^2 \) to the whole domain \( \mathbb{R}^3 \). By Eq. (3.1.44), we can obtain the following equation with chain rule for shape derivative

\[
\hat{\gamma}'(\mathbf{n}) = \nabla \hat{\gamma}(\mathbf{n}) \cdot \mathbf{n}'(\Omega; \mathbf{V})\bigg|_S = -\xi \cdot \nabla_s (\mathbf{V}_0 \cdot \mathbf{n}).
\] (3.2.1)
By the theorem, 3.1.2, and note that \( \partial_{n} \hat{\gamma}(n) = \nabla \hat{\gamma} \cdot (Dn \cdot n) = 0 \), we have

\[
dW_{int}(S; V) = -\int_{S} \xi \cdot \nabla_{s}(V_{0} \cdot n) \, dS + \int_{S} [\partial_{n} \hat{\gamma}(n) + \hat{\gamma}(n)H](V_{0} \cdot n) \, dS + \int_{\Gamma} \hat{\gamma}(n)c_{r} \cdot V_{0} \, d\Gamma
\]

\[
= -\int_{S} \xi \cdot \nabla_{s}(V_{0} \cdot n) \, dS + \int_{S} \hat{\gamma}(n)H(V_{0} \cdot n) \, dS + \int_{\Gamma} \hat{\gamma}(n)c_{r} \cdot V_{0} \, d\Gamma
\]

Now integration by parts for the first term, we have

\[
dW_{int}(S; V) = \int_{S} (\nabla_{s} \cdot \xi)(V_{0} \cdot n) \, dS - \int_{S} (\xi \cdot n)(n \cdot V_{0})H \, dS
\]

\[
- \int_{\Gamma} (\xi \cdot c_{r})(n \cdot V_{0}) \, d\Gamma + \int_{S} \hat{\gamma}(n)V_{0} \cdot nH \, dS + \int_{\Gamma} \hat{\gamma}(n)V_{0} \cdot c_{r} \, d\Gamma
\]

\[
= \int_{S} (\nabla_{s} \cdot \xi)V_{0} \cdot n \, dS + \int_{\Gamma} \left[ (\xi \cdot n)c_{r} - (\xi(n) \cdot c_{r})n \right] \cdot V_{0} \, d\Gamma
\]

\[
= \int_{S} (\nabla_{s} \cdot \xi)V_{0} \cdot n \, dS + \int_{\Gamma} c_{r}^{\gamma} \cdot V_{0} \, d\Gamma,
\]

(3.2.3)

with \( c_{r}^{\gamma} = (\xi \cdot n)c_{r} - (\xi \cdot c_{r})n \). Note here \( c_{r}^{\gamma} \) is a linear combination of \( c_{r} \) and \( n \), thus we have \( c_{r}^{\gamma} \perp \tau_{r} \) as \( c_{r} \perp \tau_{r} \), \( n \perp \tau_{r} \). Beside, we have \( V_{0} \parallel S_{sub} \) as \( T \Gamma \subset S_{sub} \). If we denote \( P_{sub} \) as the projection of vector on the substrates, then for the boundary integral \( dW_{int}(S; V) \), we can rewrite

\[
c_{r}^{\gamma} \cdot V_{0} = (P_{sub}c_{r}^{\gamma} + (I - P_{sub})c_{r}^{\gamma}) \cdot V_{0}
\]

\[
= P_{sub}c_{r}^{\gamma} \cdot V_{0} = \lambda n_{r} \cdot V_{0} = (c_{r} \cdot n_{r})(n_{r} \cdot V_{0}).
\]

Thus we can simplify Eq. (3.2.3) as

\[
dW_{int}(S; V) = \int_{S} \nabla_{s} \cdot \xi(V_{0} \cdot n) \, dS + \int_{\Gamma}(c_{r}^{\gamma} \cdot n_{r})(n_{r} \cdot V_{0}) \, d\Gamma.
\]

(3.2.4)

For the substrate energy \( W_{sub} = (\gamma_{FS} - \gamma_{V_{S}})A(\Gamma) \), a simply application of lemma. 3.1.3 in 2D, we obtain the variation of \( W_{sub} \) under the vector field \( V \)

\[
dW_{sub}(S; V) = (\gamma_{FS} - \gamma_{V_{S}}) \int_{\Gamma} V_{0} \cdot n_{r} \, d\Gamma.
\]

(3.2.5)

Now combine Eq. (3.2.4) and Eq. (3.2.5), we obtain the first variation of the total surface energies of solid-state dewetting in the direction of the vector field \( V \)

\[
dW(S; V) = \int_{S} \nabla_{s} \cdot \xi(V_{0} \cdot n) \, dS + \int_{\Gamma}(c_{r}^{\gamma} \cdot n_{r} + \gamma_{FS} - \gamma_{V_{S}})(n_{r} \cdot V_{0}) \, d\Gamma.
\]

(3.2.6)
3.3 Equilibrium

If we denote $\Omega$ as the domain enclosed by the surface $S$ and the substrate $S_{\text{sub}}$, then the equilibrium problem for solid-state dewetting can be expressed as the following minimization problem subject to the constraint that the total volume of the thin film $|\Omega|$ is a constant,

$$\min_{\Omega}(W = \int_S \gamma(n) \, dS + (\gamma_{FS} - \gamma_{VS})A(\Gamma)), \quad \text{s.t.} \quad |\Omega| = \text{const.} \quad (3.3.1)$$

We first calculate the first variation of the total volume $M = |\Omega|$. Given the initial open surface $S$ with smooth boundary $\Gamma$ on the substrate $S_{\text{sub}}$, given a transformation $T_\varepsilon$, we assume it is always satisfied that $T_\varepsilon \Gamma \subset S_{\text{sub}}$, now the total volume can be given by the divergence theorem

$$M(S) = \frac{1}{3} \int_S \mathbf{X} \cdot \mathbf{n} \, dS + \frac{1}{3} \int_{S_{\text{sub}} \cap \Omega} 0 \, dS = \frac{1}{3} \int_S \mathbf{X} \cdot \mathbf{n} \, dS. \quad (3.3.2)$$

Using (3.1.41), and integration by parts, we have

$$dM(S; \mathbf{V}) = -\frac{1}{3} \int_S \mathbf{X} \cdot \nabla_S (\mathbf{n} \cdot \mathbf{V}_0) \, dS + \frac{1}{3} \int_S \left[ \partial_n (\mathbf{X} \cdot \mathbf{n}) + \mathbf{X} \cdot \mathbf{n} \mathbf{H} \right] \mathbf{n} \cdot \mathbf{V}_0 \, dS$$

$$+ \frac{1}{3} \int_{\Gamma} (\mathbf{n} \cdot \mathbf{X}) \mathbf{V}_0 \cdot \mathbf{c}_r \, d\Gamma$$

$$= \frac{1}{3} \int_S (\nabla_S \cdot \mathbf{X}) \mathbf{n} \cdot \mathbf{V}_0 \, dS + \frac{1}{3} \int_S \mathbf{n} \cdot \mathbf{V}_0 \, dS$$

$$+ \frac{1}{3} \int_{\Gamma} \left[ (\mathbf{X} \cdot \mathbf{n}) \mathbf{c}_r - (\mathbf{X} \cdot \mathbf{c}_r) \mathbf{n} \right] \cdot \mathbf{V}_0 \, d\Gamma$$

$$= \int_S \mathbf{V}_0 \cdot \mathbf{n} \, dS + \frac{1}{3} \int_{\Gamma} \left[ (\mathbf{X} \cdot \mathbf{n}) \mathbf{c}_r - (\mathbf{X} \cdot \mathbf{c}_r) \mathbf{n} \right] \cdot \mathbf{V}_0 \, d\Gamma. \quad (3.3.3)$$

Note that $(\mathbf{X} \cdot \mathbf{n}) \mathbf{c}_r - (\mathbf{X} \cdot \mathbf{c}_r) \mathbf{n}$ is perpendicular to $\mathbf{X} \big|_\Gamma$, and $\mathbf{V}_0 \big|_\Gamma$ is parallel to the $\mathbf{X} \big|_\Gamma$, so the boundary integral integral is 0. Thus we have

$$dM(S; \mathbf{V}) = \int_S \mathbf{V}_0 \cdot \mathbf{n} \, dS. \quad (3.3.4)$$

Following the definition of equilibrium shape in 2D, we have

**Definition 3.3.1 (Equilibrium shapes).** If a open surface $S_e$ is $C^2$-hypersurface with smooth boundary $\Gamma_e$, satisfies $dW(S_e; \mathbf{V}) \equiv 0, \forall$ variation vector fields $\mathbf{V}$ satisfying

$$dW(S_e; \mathbf{V}) = \int_{\Gamma_e} \mathbf{V}_0 \cdot \mathbf{n} \, dS.$$
\( \text{d}M(S_e; V) = 0, \) then \( S_e \) is an equilibrium shape of the solid-state dewetting problem Eq. (3.3.1).

Based on the definition, we have the following lemma which give the necessary and sufficient conditions for equilibrium shape of solid-state dewetting in three dimensions.

**Lemma 3.3.1.** Assume there is an surface \( S_e \) with smooth boundary \( \Gamma_e \). Then if \( S_e \) is the equilibrium shape of the solid-state dewetting problem Eq. (3.3.1) if and only if the following conditions are satisfied

\[
\nabla_{S_e} \cdot \xi = C, \text{ on } S_e. \\
c^\gamma_r \cdot n_r + \gamma_{FS} - \gamma_{VS} = 0, \text{ on } \Gamma_e.
\]

where the constant \( C \) is determined by the total volume.

Here Eq. (3.3.5b) can be called as the anisotropic Young equation in three dimensions. For arbitrary \( x \in \Gamma_e \), denote \( \theta(x) \) as the corresponding contact angle. When the surface energy is isotropic, we have \( \xi = n \) and \( c^\gamma_r = c_r \). Thus Eq. (3.3.5b) can be reduced to

\[
\cos \theta(x) + \gamma_{FS} - \gamma_{VS} = 0, \quad \forall x \in \Gamma_e.
\]

This is directly the isotropic Young equation. For the anisotropic case, If the surface energy density is given in terms of the spherical coordinates, \( \gamma(\theta, \phi) \), by Eq. (1.1.15), and note that

\[
\xi \cdot n = \gamma, \quad c_r \cdot n_r = \cos \theta(x). \\
\xi \cdot c_r = \gamma_\theta, \quad n \cdot n_r = \sin \theta(x).
\]

Thus we can rewrite Eq. 3.3.5b into

\[
\gamma \cos(\theta(x)) - \gamma_\theta \sin(\theta(x)) + \gamma_{FS} - \gamma_{VS} = 0,
\]

which is consistent with the anisotropic Young equation in 2D, see Eq. (1.2.10).
3.4 The model

Based on Eq. (3.2.6), we know the variation of the total surface energy with respect to the surface $S$ and the contact line $\Gamma$ are given by

$$\frac{\delta W}{\delta S} = \nabla_s \cdot \xi(n), \quad \frac{\delta W}{\delta \Gamma} = (c_r \cdot n_r + \gamma_{FS} - \gamma_{VS}).$$

(3.4.1)

From the Gibbs-Thomson relation [113], the chemical potential can be defined as

$$\mu = \Omega_0 \frac{\delta W}{\delta S},$$

(3.4.2)

with $\Omega_0$ representing the atomic volume. The normal velocity of the surface is given by surface diffusion flow

$$v_n = \frac{D_s \nu \Omega_0}{k_B T_e} \nabla^2_s \mu.$$

(3.4.3)

Similar to the 2D case for the migration of contact points (Eq. (2.3.4)), the normal velocity of the contact line $\Gamma$ is given by

$$v_r = -\eta \frac{\delta W}{\delta \Gamma},$$

(3.4.4)

with $\eta$ denotes the contact line mobility.

3.4.1 The dimensionless equations

Now take the characteristic length scale and characteristic surface energy scale as $L$ and $\gamma_0$ respectively, and choose the time scale as $\frac{L^4}{B \gamma_0}$ with $B = \frac{D_s \nu \Omega_0}{k_B T_e}$. Moreover, the contact line mobility is scaled by $\frac{B}{L^3}$. Assume $S$ is a $C^1$-hypersurface in $\mathbb{R}^3$ with smooth boundary $\Gamma$, let $X$ and $X_r$ represent local parametrization of the surface $S$ and the boundary $\Gamma$ respectively. Then the sharp interface model can be described as:

$$\partial_t X = \Delta_s \mu \ n, \quad t > 0,$$

(3.4.5)

$$\mu = \nabla_s \cdot \xi, \quad \xi = \nabla \dot{\gamma}(n),$$

(3.4.6)

together with the following boundary conditions
3.4.1 The model

(1) Contact line condition

\[ \Gamma \subset S_{\text{sub}}, \quad t \geq 0, \tag{3.4.7} \]

(2) Relaxed contact angle condition

\[ \partial_t \mathbf{X}_\Gamma = -\eta \left[ \mathbf{c}_\Gamma^\top \cdot \mathbf{n}_\Gamma - \sigma \right] \mathbf{n}_\Gamma, \quad t \geq 0, \tag{3.4.8} \]

where \( \mathbf{c}_\Gamma = (\xi \cdot \mathbf{n}) \mathbf{c}_r - (\xi \cdot \mathbf{c}_r) \mathbf{n}, \mathbf{n}_\Gamma = \frac{1}{\sqrt{n_1^2 + n_2^2}} (n_1, n_2, 0), \sigma = \frac{\gamma_{VS} - \gamma_{FS}}{\gamma_0} \),

(3) Zero-mass flux condition

\[ (\mathbf{c}_r \cdot \nabla \mu) \bigg|_{\Gamma} = 0, \quad t \geq 0. \tag{3.4.9} \]

3.4.2 Mass conservation and energy dissipation

In this section, we will prove that the solid-state dewetting satisfies the properties of mass conservation and energy dissipation.

Proposition 3.4.1. Let \( \mathbf{X}(\cdot, t) \), be the exact solution of the PDEs (3.4.5), (3.4.6) with boundary conditions (3.4.8), (3.4.9), denote \( S(t) \) as the moving interface, \( \Omega(t) \) as the domain enclosed by \( S(t) \) and the substrate. Then the total volume enclosed by the surface and the substrate \( S_{\text{sub}} \) is conserved, i.e.,

\[ M(t) \equiv M(0) = \iiint_{\Omega(0)} d\mathbf{X}; \tag{3.4.10} \]

and the total energy of the thin film is decreasing during the evolution, i.e.,

\[ W(t) \leq W(t_1) \leq W(0) = \iint_{S_0} \gamma(\mathbf{n}) \, dS - \sigma A(\Gamma_0), \quad t \geq t_1 \geq 0. \tag{3.4.11} \]

Proof. From Eq. (3.3.4), replacing \( \varepsilon \) with \( t \) and noting that \( \partial_t \mathbf{X} = \mathbf{V}_0 \), we have

\[ \frac{d}{dt} M(t) = \iint_{S(t)} \partial_t \mathbf{X} \cdot \mathbf{n} \, dS = \iint_{S(t)} \Delta_s \mu \, dS = 0. \tag{3.4.12} \]

The last equality comes from the integration by parts. The boundary integral vanishes due to the boundary condition Eq. (3.4.9). Thus the total volume is conserved.
Taking derivative with respect to $t$ for the total energy, by Eq. (3.2.6), we obtain

$$\frac{d}{dt} W(t) = \iint_{S(t)} \nabla_s \cdot \left[ \nabla \gamma(n) \right] \partial_t \mathbf{X} \cdot \mathbf{n} \, dS + \int_{\Gamma(t)} (\mathbf{c}_r^\gamma \cdot \mathbf{n}_r - \sigma) (\partial_t \mathbf{X}_\Gamma \cdot \mathbf{n}_r) \, d\Gamma.$$ 

Substitute $\Delta_s \mu = \partial_t \mathbf{X} \cdot \mathbf{n}$ and $\nabla_s \cdot \xi = \mu$, we have

$$\frac{d}{dt} W(t) = \iint_{S(t)} \mu \Delta_s \mu \, dS - \eta \int_{\Gamma(t)} (\mathbf{c}_r^\gamma \cdot \mathbf{n}_r - \sigma)^2 \, d\Gamma$$

$$= - \iint_{S(t)} (\nabla_s \mu)^2 \, dS - \eta \int_{\Gamma(t)} (\mathbf{c}_r^\gamma \cdot \mathbf{n}_r - \sigma)^2 \, d\Gamma \leq 0. \tag{3.4.13}$$

The last equality comes from the integration by parts.

The proof of above proposition involves calculating the derivative of the mass or energy with respect to the time $t$. This is equivalent to calculation of the first variation by considering the time $t$ as parameter $\varepsilon$ for the perturbation. Actually, the mass conservation is satisfied due to the surface diffusion flow and zero-flux boundary condition, while the energy dissipation is straightforward is because the sharp interface model is derived based on the thermodynamic variation.
A PFEM in Three Dimensions

The initial idea of the parametric finite element method is presented by Dziuk in [44], where the author formulated the discrete numerical algorithm by assuming that the new surface $S^{m+1}$ is parameterized on the last step surface $S^m$ instead of on a fixed reference domain. This treatment could considerably simplify the numerical approximation of some surface operators, such as $\nabla_s, \Delta_s$. Thus the evolving surfaces can be generated step by step without any parameterisation of the initial surface. In recent years, the parametric finite element methods have been widely used to numerically solving some geometric equations such as the mean curvature flow, surface diffusion flow, Willmore flow and so on [6,16,17,19,20,23,24,94]. Among these methods, the most considerable works are the parametric finite element methods proposed by J.W. Barrett et al. Their methods have a good preservation of the mesh quality by automatically distributing the mesh points along the discrete polygonal surfaces. These methods can be applied to the isotropic case and anisotropic case when the surface energy is given in the form of Riemannian metric.

In this chapter, we will present the parametric finite element method for solving the sharp interface model which is derived in the last chapter (Eqs.(3.4.5),(3.4.6) with boundary conditions (Eq. (3.4.8),(3.4.9)). We start with a simple case when the surface energy is isotropic since this could help us understand the method more easily. Subsequently we will extend it to the anisotropic case when the surface
energy density is not limited to the form of Riemannian metric. When the surface energy is isotropic, the Cahn-Hoffman vector can be reduced to $\xi = n$. Besides, let $X = (X_1, X_2, X_3), n = (n_1, n_2, n_3)$, it is obvious to obtain the following expression based on the definition of surface gradient

$$D_i X_j = \delta_{ij} - n_i n_j,$$

(4.0.1)

by noting the definition of $\Delta_s$, we obtain

$$\Delta_s X_j = \sum_{i=1}^{3} D_i (-n_i n_j) = -(\nabla_s \cdot n) n_j - \nabla_s n_j \cdot n = -(\nabla_s \cdot n) n_j.$$  

(4.0.2)

In view of above equation, the dimensionless chemical potential $\mu$ can then be presented in the following form

$$\Delta_s X = -(\nabla_s \cdot n) n = -\mu n.$$  

(4.0.3)

Besides, the anisotropic co-normal vector will simultaneously reduce to the co-normal vector $c_\Gamma$.

Now let $S(t)$ denote the open surface representing the interface between the film and vapor with boundary $\Gamma(t)$. Assume $X(\cdot, t)$ is a local parameterization of $S(t)$, thus the sharp interface model for the solid-state dewetting with isotropic surface energy in three dimensions can be stated as follows,

$$\partial_t X = \Delta_s \mu n, \quad t > 0,$$

(4.0.4)

$$\mu = \mathcal{H} = -\Delta_s X \cdot n,$$

(4.0.5)

with the following boundary conditions on $\Gamma$

(1) contact line condition

$$\Gamma \subset S_{\text{sub}}, \quad t \geq 0,$$

(4.0.6)

(2) relaxed contact angle condition

$$\partial_t X_r = -\eta \left[ c_\Gamma \cdot n_r - \sigma \right] n_r, \quad t \geq 0;$$

(4.0.7)

where $n_r = \frac{P_{\text{sub}} n}{|P_{\text{sub}} n|} = \frac{1}{\sqrt{n_1^2 + n_2^2}} (n_1, n_2, 0), \sigma = \frac{\gamma_{\text{VS}} - \gamma_{\text{FS}}}{\gamma_0}, P_{\text{sub}}$ is the projection operator that maps a vector onto the tangent space of $S_{\text{sub}}$. 
4.1 Variational formulation

We assume the evolution interface $S(t)$ can be parameterized as
\[ S(t) = X(u, v, t) : U \times [0, T] \to \mathbb{R}^3. \] (4.1.1)

Therefore, the boundary $\Gamma$ is a closed plane curve and can be simultaneously considered as a parameterisation on $\partial U$, namely
\[ \Gamma(t) = X_\Gamma(u, v, t) : \partial U \times [0, T] \to \mathbb{R}^3. \] (4.1.2)

The reason we require that the surface $S(t)$ should be able to be parameterized on a reference domain $U$ is to propose the variational formulation. However, in the full-discretization scheme, this assumption is not compulsory as the discrete solutions are not defined on the reference domain.

4.1.1 For surface diffusion flow

In order to present the variational formulation for Eqs. (4.0.4),(4.0.5), we introduce the following functional space
\[ W_r(U) := \{ X \in (H^1(U))^3, X\big|_{\partial U} = \Gamma \}, \] (4.1.3)

where $\Gamma$ represents a function defined on $\partial U$. For any scalar or vector valued functions $u, v$, the inner product over surface $S$ can be given by
\[ \langle u, v \rangle_S = \iint_S u \cdot v \, dS. \] (4.1.4)

Now rewrite Eqs. (4.0.4),(4.0.5),
\[ \partial_t X \cdot n = \Delta_s \mu, \] (4.1.5a)
\[ \mu \, n = -\Delta_s X. \] (4.1.5b)
By multiplying a test function \( \phi \in H^1(S) \) for Eq. (4.1.5a), and integrating by parts from Eq. (3.1.10), we obtain

\[
0 = \int_S \partial_t \mathbf{X} \cdot \mathbf{n} \, \phi \, dS - \int_S \Delta_s \mu \phi \, dS = \int_S \partial_t \mathbf{X} \cdot \mathbf{n} \, \phi \, dS \\
+ \int_S \nabla_s \mu \cdot \nabla_s \phi \, dS - \int_S (\nabla_s \mu \cdot \mathbf{n}) \phi \mathbf{H} \, dS - \int_{\Gamma} (\nabla_s \mu \cdot \mathbf{c}_r) \phi \, d\Gamma \\
= \int_S \nabla_s \mu \cdot \nabla_s \phi \, dS. \quad (4.1.6)
\]

The last equality holds on because of the zero-mass flux boundary condition (4.0.8) and \( \nabla_s \mu \cdot \mathbf{n} = 0 \). Similarly, for Eq. (4.1.5b), we multiply a test function \( \mathbf{g} \in (H^1_0(S))^3 \) with zero values on the boundary, and integration by parts give us

\[
\int_S \mu \mathbf{n} \cdot \mathbf{g} \, dS - \int_S \nabla_s \mathbf{X} \cdot \nabla_s \mathbf{g} \, dS = 0, \quad (4.1.7)
\]

where \( \nabla_s \mathbf{X} \cdot \nabla_s \mathbf{g} = \sum_{j=1}^3 \nabla_s X_j \cdot \nabla_s g_j \).

Thus we can obtain the variational formulation for the surface diffusion flow: given the initial surface \( S(0) = \mathbf{X}(U, 0) \) with its boundary (contact line) \( \Gamma(0) \), we want to find the evolutionary surface \( S(t) \in W^1_\Gamma(U), \mu \in H^1(S) \) such that

\[
\langle \partial_t \mathbf{X} \cdot \mathbf{n}, \phi \rangle_S + \langle \nabla_s \mu, \nabla_s \phi \rangle_S = 0, \quad \forall \phi \in H^1(S), \quad (4.1.8)
\]

\[
\langle \mu, \mathbf{n} \cdot \mathbf{g} \rangle_S - \langle \nabla_s \mathbf{X}, \nabla_s \mathbf{g} \rangle_S = 0, \quad \forall \mathbf{g} \in (H^1_0(S))^3. \quad (4.1.9)
\]

Here the variational formulation is not closed as we still need to determine \( \Gamma \). In the following we will present the variational formulation for the contact line migration, from which we can obtain \( \Gamma \).

### 4.1.2 For contact line migration

The contact line migration is given by Eq. (4.0.7), which describes the motion of a plane curve on the substrate. To obtain a variational formulation for the contact line migration, we begin by adding a small regularization term

\[
\partial_t \mathbf{X}_r = \varepsilon^2 \partial_{ss} \kappa \mathbf{n}_r - \eta [\mathbf{c}_r \cdot \mathbf{n}_r - \sigma] \mathbf{n}_r, \quad t \geq 0. \quad (4.1.10)
\]
4.1 Variational formulation

Here $s$ is the arc length of the plane curve $\Gamma$, $\varepsilon$ is a small regularization parameter, and $\kappa$ is the curvature. In addition, for scalar or vector valued functions $u, v$, we define the $L^2$ inner product over $\Gamma$

$$\langle u, v \rangle_{\Gamma} = \int_{\Gamma} u \cdot v \, ds.$$  \hspace{1cm} (4.1.11)

Then a variational formulation for Eq. (4.1.10) can be stated as following: given the initial plane curve $\Gamma(0) = X_{\tau}(\partial U, 0)$, for any time $t \in (0, T]$, find the evolution curves $\Gamma(t) = X_{\tau}(\partial U, t) \in (H^1(\partial U))^3$, $\kappa \in H^1(\Gamma)$ such that

$$\langle \partial_t X_{\tau} \cdot n_{\tau}, \varphi \rangle_{\Gamma} + \varepsilon^2 \langle \partial_s \kappa, \partial_s \varphi \rangle_{\Gamma} = -\eta \langle c_{\tau} \cdot n_{\tau} - \sigma, \varphi \rangle_{\Gamma}, \quad \forall \varphi \in H^1(\Gamma), \quad (4.1.12a)$$

$$\langle \kappa, n_{\tau} \cdot \omega \rangle_{\Gamma} - \langle \partial_s X_{\tau}, \partial_s \omega \rangle_{\Gamma} = 0, \quad \forall \omega \in (H^1(\Gamma))^3, \quad (4.1.12b)$$

with $\Gamma = \Gamma(t)$. Eq. (4.1.12a) is obtain by writing the Eq. (4.1.10) in the form

$$\partial_t X_{\tau} \cdot n_{\tau} = \varepsilon^2 \partial_{ss} \kappa - \eta \left[ c_{\tau} \cdot n_{\tau} - \sigma \right],$$  \hspace{1cm} (4.1.13)

then multiplying the test functions $\varphi$ and integrating by parts with periodic boundary conditions. Similarly, Eq. (4.1.12b) is obtained by presenting the curvature in the form $\kappa n = -\partial_{ss} X_{\tau}$. The advantage of adding this small surface diffusion flow regularization for the contact line migration is that we can propose a nice variational formulation for the motion of the contact line based on the work by J. W. Barrett [16]. Besides, the fully discrete scheme based on this variational formulation tends to distribute the mesh points uniformly according to the arc length, which is helpful to increase the total mesh quality [8, 16]. In most cases, the initial contact line is given as a closed curve which is only piecewise smooth with some sharp corners. This small surface diffusion regularization can help to round the corner after several steps evolution, thus avoiding ear formulation. Note here $c_{\tau}$ in Eq. (4.1.12a) is dependent on the surface $S(t)$.

4.1.3 Mass conservation and energy dissipation

Proposition 4.1.1 (Mass conservation for weak solution). Let $(X(u, v, t), \mu(S, t))$ be a weak solution for the above variational problem Eq. (4.1.8),(4.1.9),(4.1.12a)
and (4.1.12b), then the total volume enclosed by the surface and the substrate is conserved, i.e.,

\[ M(t) \equiv M(0) = \iiint_{\Omega(0)} dX, \quad t \geq 0. \]  

(4.1.14)

**Proof.** It is easy to obtain that

\[ \frac{d}{dt}M(t) = -\int_{S} \partial_t X \cdot n \ dS. \]  

(4.1.15)

Let \( \phi = 1 \) in Eq. (4.1.8), we have \( \frac{d}{dt}M(t) = 0 \). This immediately indicates that the total volume is conserved.

\( \square \)

**Proposition 4.1.2.** Let \((X(u,v,t), \mu(S,t))\) be a weak solution for the above variational problem Eq. (4.1.8), (4.1.9), (4.1.12a) and (4.1.12b). If we assume that the surface has high regularity, that is \( X(u,v,t) \in C^1(C^2(U), [0,T]) \) and the contact line \( X_\Gamma(\partial U, t) \in C^1(C^2(\partial U), [0,T]) \), then the total energy of the system is decreasing, i.e.,

\[ W(t) \leq W(t_1) \leq W(0) \equiv \iiint_{S(0)} dS - \sigma A(\Gamma(0)), \quad t \geq t_1 \geq 0. \]  

(4.1.16)

**Proof.** Taking derivative of the total energy with respect to the time \( t \), based on Eq. (3.1.38), Eq. (3.2.5), and noting that \( V_0 = \partial_t X \), we have the following

\[ \frac{d}{dt}W(t) = \iiint_{S} \nabla S X \cdot \nabla S (\partial_t X) \ dS - \sigma \int_{\Gamma} \partial_t X_\Gamma \cdot n_r \ d\Gamma. \]  

(4.1.17)

Besides, for arbitrary vector \( V \), we have

\[ \nabla_s X \cdot \nabla_s V = \sum_{i=1}^{3} \sum_{j=1}^{3} D_j X_i D_j V_i = \sum_{i=1}^{3} \sum_{j=1}^{3} (\delta_{ij} - n_i n_j) D_j V_i \]

\[ = \sum_{i=1}^{3} \sum_{j=1}^{3} \delta_{ij} D_j V_i - \sum_{i=1}^{3} \sum_{j=1}^{3} n_i n_j D_j V_i \]

\[ = \sum_{i=1}^{3} D_i V_i - \sum_{i=1}^{3} n_i n \cdot \nabla_s V_j = \nabla_s \cdot V. \]  

(4.1.18)

Thus we can rewrite Eq. (4.1.17) as

\[ \frac{d}{dt}W(t) = \iiint_{S} \nabla_s X \cdot \nabla_s (\partial_t X) \ dS - \sigma \int_{\Gamma} \partial_t X_\Gamma \cdot n_r \ d\Gamma. \]  

(4.1.19)
4.1 Variational formulation

As the surface $S$ and the contact line $\Gamma$ are parametrized on the reference domain $U$ and $\partial U$ respectively, if the test function is defined on $S$ or $\Gamma$, we can also regard it as a parametrization on $U$ or $\partial U$. Now for fixed $\delta$, there exist a closed domain $V$ belongs to the reference domain $U$ such that the measure $m(U/V) < \delta$, and choose the test function $g$ in Eq. (4.1.9) such that $g|_V = \partial_t X|_V$, and $g|_{\partial U} = 0$, also let $\varphi = \mu$ in Eq. (4.1.8), we obtain

$$\langle \nabla_s X, \nabla_s (\partial_t X - g) \rangle_S$$

$$= \langle \nabla_s X, \nabla_s (\partial_t X - g) \rangle_S + \langle \nabla_s X, \nabla_s g \rangle_S$$

$$= \langle \nabla_s X, \nabla_s (\partial_t X - g) \rangle_S + \langle \mu, n \cdot g \rangle_S$$

$$= \langle \nabla_s X, \nabla_s (\partial_t X - g) \rangle_S + \langle \mu, n \cdot \partial_t X \rangle_S + \langle \mu, n \cdot (g - \partial_t X) \rangle_S$$

$$= \langle \nabla_s X, \nabla_s (\partial_t X - g) \rangle_S - \langle \nabla_s \mu, \nabla_s \mu \rangle_S + \langle \mu, n \cdot (g - \partial_t X) \rangle_S. \quad (4.1.20)$$

The regularity of the surface ensures that we can perform integration by parts for the first term of above equation,

$$\langle \nabla_s X, \nabla_s (\partial_t X - g) \rangle_S = \langle (\partial_t X - g), n \cdot (\nabla_s \cdot n) \rangle_S + \langle (\partial_t X - g), c_r \cdot \Gamma \rangle.$$ \quad (4.1.21)

Thus we obtain that

$$\frac{d}{dt} W(t) = \langle (\mu + \nabla_s \cdot n) \cdot (g - \partial_t X) \rangle_S$$

$$- \langle \nabla_s \mu, \nabla_s \mu \rangle_S + \langle \partial_t X_r \cdot n_r, c_r \cdot n_r - \sigma \rangle \Gamma. \quad (4.1.22)$$

Now let $\varphi = c_r \cdot n_r - \sigma$ in Eq. (4.1.12a), we obtain that

$$\frac{d}{dt} W(t) = \langle (\mu - \nabla_s \cdot n) \cdot (g - \partial_t X) \rangle_S - \varepsilon^2 \langle \partial_s \kappa, \partial_s (c_r \cdot n_r) \rangle \Gamma$$

$$- \langle \nabla_s \mu, \nabla_s \mu \rangle_S - \eta \langle c_r \cdot n_r - \sigma, c_r \cdot n_r - \sigma \rangle \Gamma. \quad (4.1.23)$$

By the definition of $g$, the first term can be as small as possible and bounded by $C\delta$. The second term can be bounded by the last term for smaller enough $\varepsilon$. So this indicates that $\frac{d}{dt} W(t) \leq 0. \qquad \Box$
4.2 Spatial/temporal discretization

Based on the variational formulation Eq. (4.1.8), (4.1.9), (4.1.12a) and (4.1.12b), in this section, we introduce the fully discrete scheme. We first divide the time as

$$0 = t_1 < t_2 < \ldots < t_M = T,$$

with time step $$\tau_m = t_{m+1} - t_m$$. In the spatial level, let

$$S^m = \bigcup_{j=1}^{N} \bar{D}^m_j,$$

where $$\{D^m_j\}_{j=1}^{N}$$ are mutually disjoint triangle surfaces, (4.2.2)

be a polygonal surface approximating the evolution surface $$S(t_m)$$ for $$1 \leq m \leq M$$. Assume the polygonal surface has $$K$$ vertices given as $$\{q^m_k\}_{k=1}^{K}$$. The boundary of the polygonal surface $$S^m$$ is a polygonal curve $$\Gamma^m$$, which can be expressed as

$$\Gamma^m = \bigcup_{j=1}^{N_c} \bar{h}^m_j,$$

where these line segments are ordered in anti-clockwise direction when viewing from the top. We use the $$P^1$$ finite elements, that means the function is linear on every element. Therefore we can define the following finite element spaces on $$S^m$$ and $$\Gamma^m$$

$$\mathcal{V}^h(\Gamma^m) := \{ \phi \in C(\Gamma^m, \mathbb{R}) : \phi \bigg|_{h^m_j} \text{ is linear } \forall 1 \leq i \leq N_c \} \subset H^1(\Gamma^m).$$

$$\mathcal{V}^h(S^m) := \{ \phi \in C(S^m, \mathbb{R}) : \phi \bigg|_{D^m_j} \text{ is linear } \forall 1 \leq i \leq N \} \subset H^1(S^m).$$

Besides, we can define the finite element space on $$S^m$$ with zero values on $$\Gamma^m$$

$$\mathcal{V}^h_0(S^m) := \{ \phi \in \mathcal{V}^h(S^m), \phi \bigg|_{h^m_k} = 0, \forall 1 \leq k \leq N_c \} \subset H^1_0(S^m).$$

If we assume $$\Gamma^h := X_{\Gamma^h} \in (\mathcal{V}^h(\Gamma^m))^3$$, then we can define the space on $$S^m$$ such that the boundary is given as $$\Gamma^h$$, that is

$$\mathcal{W}^h_{\Gamma^h} = \{ g \in C(S^m, \mathbb{R}^3) : g \in (\mathcal{V}^h(S^m))^3, g \bigg|_{\Gamma^m} = X_{\Gamma^h} \}.$$ 

The polygonal surface $$S^m$$ consists of $$N$$ triangle surfaces $$\{D^m_j\}_{j=1}^{N}$$ in three dimensions, see Fig. 4.1(a). If we assume that $$\{q^m_{j1}, q^m_{j2}, q^m_{j3}\}$$ are the vertices of the
4.2 Spatial/temporal discretization

Fig. 4.1: Typical triangles in the mesh. (a) A triangle with no edges on the boundary. (b) Two connected triangles with edges on the boundary.

In addition, as the boundary of the surface $S^m$, $\Gamma^h$ is a plane curve on the substrate ($xOy$ plane), which consists of connected line segments, see Fig. 4.1(b) (colored in blue). Here we assume that $\{p_{j,1}^m, p_{j,2}^m\}$ are the two vertices of $h_j^m$ and ordered in the anti-clockwise direction viewing from the positive $z$ axis direction. Let $n_{r,m}$ denote the unit normal vector of $\Gamma^m$ on the substrate, then it is also a step function with discontinuities on the endpoints of each line segment $h_j^m$. If $n_{r,m,j}$ is the normal function of $\Gamma^m$ on line segment $h_j^m$, then

$$n_{r,m,j} = n_{r,m}\bigg|_{h_j^m} = \frac{(p_{j,2}^m - p_{j,1}^m) \times z}{|p_{j,2}^m - p_{j,1}^m| \times z|} \quad \forall 1 \leq j \leq N_c,$$

(4.2.8)

where $z$ is the unit vector along the positive direction of $z$ axis. Now we can define the following mass-lumped norms to approximate the integration on $S^m$ or
\[ \Gamma^m \text{ respectively,} \]
\[
\langle u, v \rangle_{\Gamma_m} = \frac{1}{3} \sum_{j=1}^{N} |D_j^m| \sum_{k=1}^{3} u((a_k^m)^-) \cdot v((a_k^m)^-). 
\]
\[
\langle f, g \rangle_{\Gamma_m} = \frac{1}{2} \sum_{j=1}^{N} |h_j^m| \sum_{k=1}^{2} f((p_k^m)^-) \cdot g((p_k^m)^-). 
\]

Here in this expressions, \(|D_j^m|, |h_j^m|\) are the area of the triangle of \(D_j^m\) and length of \(h_j^m\) respectively. \(u, v\) are two scalar or vector functions defined on \(S^m\). \(f, g\) are two scalar or vector functions defined on \(\Gamma^m\). Since the integrand could be discontinuous functions, thus we define \(u((a_k^m)^-)\) as the limit of \(u(x)\) when \(x\) approaches towards \(a_k^m\) from triangles \(D_j^m\), and \(f((p_k^m)^-)\) as the limit of \(f(x)\) when \(x\) approaches towards \(p_k^m\) from the line segment \(h_j^m\).

Finally we propose the following approximation of the variational formulation Eqs. (4.1.12a),(4.1.12b),(4.1.8) and (4.1.9): assume \(S^0 = \bigcup_{j=1}^{N} D_j^0\) is a discretization of the initial surface \(S(0)\) with good mesh quality, and \(\Gamma^0 = \bigcup_{j=1}^{N} \Gamma_j^0\), for \(1 \leq m \leq M - 1\), we want to find \(S^{m+1} := X^{m+1} \in W_{\Gamma_m+1}(S^m), \mu^{m+1} \in V^h(S^m)\), such that

\[
\langle X^{m+1} - X^m, n^m, \phi_h \rangle_{S_m} + \langle \nabla S \mu^{m+1}, \nabla S \phi_h \rangle_{S_m} = 0, \quad \forall \phi_h \in V^h(S^m), \quad (4.2.9a)
\]
\[
\langle \mu^{m+1}, n^m \cdot \phi_h \rangle_{S_m} - \langle \nabla S X^{m+1}, \nabla S \phi_h \rangle_{S_m} = 0, \quad \forall \phi_h \in (V_0(S^m))^3, \quad (4.2.9b)
\]

where \(\Gamma^{m+1}\) can be found by the following approximation: find \(\Gamma^{m+1} := X_{\Gamma_m+1} \in (V^h(\Gamma^m))^3, \kappa^{m+1} \in V^h(\Gamma^m)\), such that

\[
\langle X_{\Gamma_m+1} - X_{\Gamma_m}, n_{\Gamma_m}, \phi_h \rangle_{\Gamma_m} + \varepsilon^2 \langle \partial_s \kappa^{m+1}, \partial_s \phi_h \rangle_{\Gamma_m} + \eta \langle c_{\Gamma_m} \cdot n_{\Gamma_m} - \sigma, \phi_h \rangle_{\Gamma_m} = 0, \quad \forall \phi_h \in V^h(\Gamma^m), \quad (4.2.10a)
\]
\[
\langle \kappa^{m+1}, n_{\Gamma_m} \cdot \omega_h \rangle_{\Gamma_m} - \langle \partial_s X_{\Gamma_m+1}, \partial_s \omega_h \rangle_{\Gamma_m} = 0, \quad \forall \omega_h \in (V^h(\Gamma^m))^3. \quad (4.2.10b)
\]

We note that in the above discrete scheme, we use the semi-implicit parametric finite element method instead of the fully implicit parametric finite element method. The integrations are calculated on \(S^m\) and \(\Gamma^m\). Besides, all the nonlinear terms such as \(n^m\) and \(n_{\Gamma_m}\) are valued explicitly. For each time step, we first update the boundary \(\Gamma^{m+1}\) by solving Eqs. (4.2.10a),(4.2.10b). In this scheme, \(c_{\Gamma_m}\) is the unit
4.2 Spatial/temporal discretization

co-normal vector of the polygonal surface on the boundary, which is a step function on \( \Gamma^m \). We can numerically value it as

\[
c_{\Gamma^m,j} = \frac{(p_{j2}^m - p_{j1}^m) \times n_{kj}^m}{|p_{j2}^m - p_{j1}^m|},
\]

where \( p_{j1}^m, p_{j2}^m \) are the vertices of the line segment \( h_j^m \) and ordered in the anticlockwise direction. \( n_{kj}^m \) is the unit outer normal vector of the triangle surface \( D_{kj}^m \) which contains the line segment \( h_j^m \). After this, we can obtain \( S^{m+1} \) from Eqs. (4.2.16a),(4.2.10b). By considering that \( S^{m+1} \) is parametrized on \( S^m \) and \( \Gamma^{m+1} \) is parametrized on \( \Gamma^m \), the term \( \nabla_S \) and \( \partial_s \) operators can be easily calculated, which demonstrates the essential convenience of parametric finite element method.

Precisely, consider triangle surface \( D_j^m \) with vertices \( \{q_{j1}^m, q_{j2}^m, q_{j3}^m\} \) ordered in the anticlockwise direction from the outside of the surface, then we have

\[
\nabla_S B_i(S^m) \bigg|_{D_j^m} = \frac{(q_{j3}^m - q_{j2}^m) \times n_{j}^m}{2|D_j^m|},
\]

where \( B_i \) is the nodial basis function at point \( q_{ji}^m \). Thus for any arbitrary function \( \phi \in \mathcal{V}^h(S^m) \), we can derive

\[
\nabla_S \phi \bigg|_{D_j^m} = \sum_{i=1}^3 \phi(q_{j1}^m) \nabla_S B_i.
\]

Similarly, for any arbitrary function \( \varphi \in \mathcal{V}^h(\Gamma^m) \), we also have

\[
\partial_s \varphi \bigg|_{h_j^m} = \frac{\varphi(p_{j1}^m) - \varphi(p_{j2}^m)}{|h_j^m|}.
\]

The numerical approximation of the geometric operator \( \nabla_S, \partial_s \) becomes easier, and the discrete numerical approximations turn out to be two linear systems. We have the following theorem for the well-posedness of the scheme.

**Theorem 4.2.1.** [Well-posedness of the PFEM scheme] The discrete variational problems, Eqs. (4.2.16a), (4.2.16b), (4.2.10a) and (4.2.10b) is well-posed.

**Proof.** To prove the well-posedness of the PFEM scheme, we need prove the linear system obtained from
4.2 Spatial/temporal discretization

Eqs. (4.2.10a), (4.2.10b) both have unique solution. It is equivalent to prove the two corresponding homogenous linear systems only have zero solutions. To solve $\Gamma^{m+1}$, we prove the following system has zero solution.

$$\langle X_{\Gamma^{m+1}} \cdot n_{\Gamma^m}, \varphi_h \rangle_{\Gamma^m} + \tau_m \langle \partial_s (X_{\Gamma^{m+1}}), \partial_s \varphi_h \rangle_{\Gamma^m} = 0, \forall \varphi_h \in V_h(\Gamma^m),$$

(4.2.15a)

$$\langle \kappa_{m+1}, n_{\Gamma^m} \cdot \omega_h \rangle_{\Gamma^m} - \langle \partial_s X_{\Gamma^{m+1}}, \partial_s \omega_h \rangle_{\Gamma^m} = 0, \forall \omega_h \in (V_h(\Gamma^m))^3.$$

(4.2.15b)

By choosing $\omega_h = X_{\Gamma^{m+1}}, \varphi = \kappa_{m+1}$, it is easy to prove that $X_{\Gamma^{m+1}} = 0, \kappa_{m+1} = 0$ is the solution, see [16].

For the linear system of Eqs. (4.2.16a), (4.2.16b), the corresponding homogenous linear system is to find $X^{m+1} \in (V_h^0(S^m))^3, \mu \in V_h^0(S^m)$

$$\langle X^{m+1} \cdot n^m, \phi_h \rangle_{S^m} + \tau_m \langle \nabla_s (X^{m+1}), \nabla_s \phi_h \rangle_{S^m} = 0, \forall \phi_h \in V_h(S^m),$$

(4.2.16a)

$$\langle \mu^{m+1}, n^m \cdot g_h \rangle_{S^m} - \langle \nabla_s X^{m+1}, \nabla_s g_h \rangle_{S^m} = 0, \forall g_h \in (V_h^0(S^m))^3.$$

(4.2.16b)

By choosing $\phi = \mu^{m+1}, g_h = X^{m+1}$, we can obtain

$$\tau_m \langle \nabla_s (\mu^{m+1}), \nabla_s X^{m+1} \rangle_{S^m} + \langle \nabla_s X^{m+1}, \nabla_s X^{m+1} \rangle_{S^m} = 0.$$  

(4.2.17)

Thus we obtain $X^{m+1} = 0$ by the zero boundary, and then $\mu^{m+1} = 0$. So we have proved the uniqueness and existence of the two linear systems obtained from the scheme, thus the semi-implicit PFEM scheme is well-posed.

To summarise, our parametric finite element method is a combination of the parametric finite element method for closed curve evolution [16] (the contact line migration by a small surface diffusion regularization) and the parametric finite element method for open surface [20] (interface evolution under surface diffusion flow). The mesh quality can be preserved such that there is no need to do any mesh regularizations during the evolution as long as the initial mesh quality is good enough. The two linear systems obtained from the PFEM scheme can be solved via Spare LU decomposition. The mass matrix under the mass-lumped norm can be reduced to the simple diagonal matrix, thus the linear systems are easy to be solved even though the mass matrix and stiffness matrix are dependent on the time step.
4.3 Numerical results

In this section, based on the PFEM scheme, we will show some numerical results for the scheme.

4.3.1 Contact line mobility and smooth effect

From the relaxation boundary condition in Eq. (4.0.7), which controls the migration of the contact line, we know that the mobility precisely represents the relaxation rate of the contact angle towards the equilibrium contact angle. The large \( \eta \) will accelerate the relaxation process \([120]\). Thus the choice of \( \eta \) will have significant influence on the dynamic evolution of the surface, especially the contact angles of the surface. On the other hand, \( \eta \) is a material parameter and could be variant for different materials. Therefore, we will numerically investigate the effect of \( \eta \) on the evolution of the dynamic contact angles firstly. For the polygonal surface, we define the following indicator,

\[
\bar{\theta}^m = \frac{1}{N_c} \sum_{j=1}^{N_c} \arccos(c_{r_{m,j}} \cdot n_{r_{m,j}}),
\]

(4.3.1)

which is the mean value of all the contact angles on each line segment of \( \Gamma^m \). Fig. 4.2 shows the temporal evolution of \( \bar{\theta}^m \) and the normalized energy \( W(t)/W(0) \) under different choices of the mobility. The initial thin film is chosen as a unit cube on the substrate with material constant \( \sigma = \cos(3\pi/4) \). From the figure, we can observe that the larger mobility will accelerate the process of relaxation such that the contact angles evolve faster towards the same equilibrium angle \( \frac{3\pi}{4} \). Similarly, as shown in Fig. 4.2(b), the energy decays faster for larger mobility, but finally reaches the same value. This indicates that the equilibrium contact angles as well as the equilibrium shape are independent on the choice of \( \eta \). So in the following, without special mention, we always assume the mobility is chosen as \( \eta = 100 \).

As discussed previously, the introduction of the smooth regularization for the contact line migration enables us to apply PFEM to approximate the contact line
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Figure 4.2: (a) The temporal evolution of contact angle $\bar{\theta}_m$ defined in Eq. (4.3.1); (b) the temporal evolution of the normalized energy $W(t)/W(0)$ for different choices of mobility.

Figure 4.3: Comparison of the dynamic contact lines under different regularization parameter $\epsilon$. The initial thin film is a cuboid with dimension $(3.2, 3.2, 0.1)$. The computational parameter is chosen as $\eta = 100, \sigma = \cos(5\pi/6)$. 
4.3 Numerical results

migration. It is obvious that the smaller regularization parameter $\varepsilon$ is desired. However, numerical mesh size, as well as the time step, prevents us from choosing too small $\varepsilon$. Fig. 4.3 shows the geometric comparison of the contact lines for different $\varepsilon$ at time $t = 0.02, 0.12, 0.52$. The initial thin film is given by a $(3.2, 3.2, 0.1)$ cuboid with computational parameter chosen as $\eta = 100, \sigma = \cos(5\pi/6)$. From the figure, we can observe that when $\varepsilon \leq 0.01$, the influence of the regularization on the contact line migrations could be almost ignored. Thus, it is always assumed the regularization parameter is chosen as $\varepsilon = 0.01$ if there is no special mention. On the other hand, our numerical simulations demonstrate that when $\varepsilon$ is too big, this regularization could be regarded as a drag effect and will cause the mesh deterioration.

4.3.2 Convergence test

![Mesh refinement procedure](image.png)

Figure 4.4: A illustration of mesh refinement procedure by dividing each triangle into four small triangles.

For an initial cuboid, we assume each face of the cuboid except the face on the substrate consists of squares and each square is divided into 4 triangles. Based on this mesh, we can refine it by dividing each right triangle into four small ones, see Fig. 4.4. This mesh refinement procedure can be then repeated to produce the mesh with desirable mesh size. For the initial polygonal mesh, we can define mesh size $h$ as the length of the hypotenuse of the small right triangles. Thus for a mesh obtained via $n$ refinements, one can immediately get $h = \frac{1}{2^n}$. 
4.3 Numerical results

We firstly want to investigate the convergence of our PFEM for the equilibrium shape. Fig. 4.5 and Fig. 4.6 show the convergence of the cross-section profiles and contact lines respectively. For mesh1, the initial polygonal mesh is obtained after 3 refinements with $h = 0.125$, and the time step is chosen as $\tau_1 = 1.25 \times 10^{-3}$. As mesh2 is a refinement of mesh1 and mesh3 is a refinement of mesh2, thus the time step for them is chosen as $\frac{\tau_1}{4}$ and $\frac{\tau_1}{16}$. The two figures clearly demonstrate that the numerical equilibrium shape is convergence towards the theoretical equilibrium shape as the mesh size decreases.

Figure 4.5: Comparison of the cross-section profiles in $x$-direction of the numerical equilibrium shapes for different meshes with that of the theoretical equilibrium shape. The initial surface is a unit cube on the substrate, $\sigma = \cos(15\pi/36)$.

To our knowledge there is no theory for the convergence order of the PFEM scheme so far, but it is still interesting to investigate the convergence of the scheme. Given the numerical polygonal surface $X^m$ at discrete time $t_m$ with $0 \leq m \leq M$, we can define the numerical solution at arbitrary time $t_m \leq t < t_{m+1}$ as a linear interpolation

$$X_{h,\tau}(t) = \frac{t_{m+1} - t}{\tau_m} X^m + \frac{t - t_m}{\tau_m} X^{m+1}. \tag{4.3.2}$$

Here $h$ is the mesh size of the $X^0$, $\tau$ is the uniform time step. Since there is no analytical solution for us to compare with our numerical solution, we define the
4.3 Numerical results

Figure 4.6: Comparison of the numerical contact lines of the equilibrium shapes for different meshes with the contact line of the theoretical equilibrium shape. The initial surface is a unit cube on the substrate, \( \sigma = \cos(15\pi/36) \).

The numerical error as following

\[
e_{h,\tau}(t) = \|X_{h,\tau}(t) - X_{h,\tau}(t)\|_{L^\infty} = \max_{1 \leq k \leq K} \min_{1 \leq j \leq N} \text{dist}(q_k, D_j),
\]

where \( q_j \) is the vertices of \( X_{h,\tau} \), and \( D_j \) is the triangle of \( X_{h,\tau}(t) \). dist is the distance function for a vertices to a triangle in three dimensions. In order to test the convergence order, the computation set-up is prepared as following: the initial thin film is chosen as a cuboid with dimension \( (1, 2, 1) \). The material constant is fixed with \( \sigma = \cos(3\pi/4) \), and \( h_0 = 0.5, \tau_0 = 0.005 \). We compute the convergence order at three different time \( t = 0.02, 0.05, 0.1 \).

From Table. 4.1, we can observe the convergence order is around 1. The convergence test for the PFEM applied to mean curvature flow with closed surface has been reported in [20] and the convergence order is 2. Here the convergence order for our PFEM reduces to 1. The reason may be due to our explicit scheme for the contact line migration.
Table 4.1: Convergence rates in the $L^\infty$ norm for an open surface evolution under the isotropic surface diffusion flow (solid-state dewetting with isotropic surface energy), where the computational parameters are chosen as: $\sigma = \cos(3\pi/4)$. The initial thin film is given as a $(1, 2, 1)$ cuboid.

<table>
<thead>
<tr>
<th>$e_{h,\tau}(t)$</th>
<th>$h = h_0$</th>
<th>$h_0/2$</th>
<th>$h_0/2^2$</th>
<th>$h_0/2^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau = \tau_0$</td>
<td></td>
<td>$\tau_0/2^2$</td>
<td>$\tau_0/2^4$</td>
<td>$\tau_0/2^6$</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 0.02)$</td>
<td>1.13E-1</td>
<td>3.63E-2</td>
<td>1.34E-2</td>
<td>5.90E-2</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>1.63</td>
<td>1.43</td>
<td>1.18</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 0.05)$</td>
<td>1.14E-1</td>
<td>4.16E-2</td>
<td>1.72E-2</td>
<td>8.40E-2</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>1.45</td>
<td>1.27</td>
<td>1.03</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 0.10)$</td>
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<td>4.23E-2</td>
<td>2.00E-2</td>
<td>1.01E-2</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>1.24</td>
<td>1.08</td>
<td>0.99</td>
</tr>
</tbody>
</table>

4.3.3 Small islands

Fig. 4.7 shows several stages of the evolution of a unit cube towards its equilibrium shape. The initial mesh consists of 1280 same right triangles with two legs sharing the same length of $\sqrt{2}$. The mesh contains 657 vertices with 32 vertices on the boundary. We can observe that the unit cube finally evolves into a spherical geometry with contact angle approximating $3\pi/4$.

Fig. 4.8(a) shows the temporal evolution of the normalized mass and energy, where the computational parameter is chosen the same as Fig. 4.7. As is shown in the figure, the mass conservation and energy dissipation is clearly demonstrated, which indicates the discrete PFEM scheme can grasp these fundamental properties of solid-state dewetting. Fig. 4.8(b) depicts the logarithm of the mesh distribution function $\psi(t)$ during the time evolution, where $\psi(t)$ is the indicator of the mesh quality defined as

$$\psi(t_m) = \frac{\max_{j=1}^N |D_j^m|}{\min_{j=1}^N |D_j^m|}.$$  (4.3.4)
4.3 Numerical results

Figure 4.7: Several snapshots in the evolution of a small initially unit cube towards its equilibrium shape with parameter chosen as $\sigma = \cos(3\pi/4)$, (a) $t = 0$; (b) $t = 2e - 4$; (c) $t = 0.02$; (d) $t = 0.2$.

Figure 4.8: (a) The temporal evolution of the normalized total free energy and the normalized volume (mass); (b) the temporal evolution of the logarithm of the mesh distribution function $\psi(t)$. The computational parameter is chosen as same as Fig. 4.2.
From the figure, it can be seen that $\ln(\psi(t))$ is bounded and tends to be horizontal as time evolves, which indicates that our PFEM scheme has a good mesh quality preservation. Thus mesh regularization is not needed during the computation.

The influence of the material constant $\sigma$ on the equilibrium shape has been investigated and the result is shown in Fig. 4.9. It clearly demonstrates that the $\sigma$ determines the contact angle of the equilibrium shape.

![Figure 4.9](image)

Figure 4.9: The equilibrium shape of an initial unit cube with different material constants $\sigma$.

### 4.3.4 Large islands

If the initial thin film is given by long thin islands, it possibly breaks up into small islands due to the Rayleigh instability [84, 99]. Therefore, we want to investigate the evolution of long islands with dimensions $(1, m, 1)$. We test three examples with $m = 4, 12, 16$, and the material constant is fixed with $\sigma = \cos(3\pi/4)$. As depicted in Fig. 4.10, the thin film with dimension $(1, 4, 1)$ evolves and forms a single island with spherical geometry. When we choose larger $m$, the thin films break up into 2 small islands or 3 smalls islands, see Fig. 4.11 and Fig. 4.12 respectively.

In order to fully understand the geometry evolution for the thin film, we have depicted several snapshots for the contact lines and cross-section profiles for the thin film, see Fig. 4.13. From the figure, we can observe that the thin films pinch off at a point, where both the contact line and cross-section profiles break up.
Figure 4.10: Several snapshots in the evolution of an initial cuboid with dimension (1, 4, 1) towards its equilibrium. (a) $t = 0$; (b) $t = 0.01$; (c) $t = 0.10$; (d) $t = 2.35$. The computational parameter is chosen as $\sigma = \cos(3\pi/4)$.

Figure 4.11: Several snapshots in the evolution of an initial cuboid with dimension (1, 12, 1) until its pinch off. (a) $t = 0$; (b) $t = 0.01$; (c) $t = 0.50$; (d) $t = 1.07$. The computational parameter is chosen as $\sigma = \cos(3\pi/4)$. 
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Figure 4.12: Several snapshots in the evolution of an initial cuboid with dimension $(1, 16, 1)$ until its pinch off. (a) $t = 0$; (b) $t = 0.20$; (c) $t = 0.75$; (d) $t = 1.14$. The computational parameter is chosen as $\sigma = \cos(3\pi/4)$.

Then there must exist critical lengths $L_1, L_2$, such that when $L_1 \leq m \leq L_2$, the long thin film breaks up into 2 small isolated islands, and when $L \geq L_2$, the long thin film breaks up into 3 or more than 3 small isolated islands. Besides, these two critical lengths should be dependent on the material constant $\sigma$. We give the phase diagrams for the numbers of islands formed from the initially $(1, L, 1)$ cuboid islands with material constant $\sigma$ in Fig. 4.14(a). From the figure, we can observe that for the long islands, the critical length $L_1$ and $L_2$ are linear to $\frac{1}{\sin(\arccos \sigma/2)}$. This relation has been observed and reported in two dimensions both for isotropic and weakly anisotropic surface energy [40,120]. Moreover, we also plot the pinch-off time $t_p$ for $(1, L, 1)$ cuboid island for $\sigma = \cos \frac{\pi}{3}, \cos \frac{\pi}{2}, \cos \frac{2\pi}{3}$. From the figure, we can observe, at the beginning, as $L$ increases, the time the thin film pinches off increasing quickly as a consequence. However, as $L$ reaches the critical length $L_2$, the line for pinch-off time drops and then almost stays horizontal.

We consider the morphology evolutions of large thin films with dimensions $(m, m, 1)$. We start by simulating the evolution of an initial square with dimensions $(3.2, 3.2, 0.1)$,
Figure 4.13: Several snapshots in the evolution of the contact lines (shown in column (a)) and the cross-section profile (shown in column (b)) until pinch off. The computational parameter is chosen as $\sigma = \cos(3\pi/4)$. 
Figure 4.14: (a) Phase diagram for the number of islands formed from the initial (1, L, 1) cuboid with material constant $\sigma$. The boundaries are given by our fitting linear curve $L = 3.98 + 4.64x$ and $L = 6.84 + 6.725x$, where $x = \frac{1}{\sin(\frac{\cos^{-1} \sigma}{2})}$. (b) The pinch off time $t_p$ for the initial (1, L, 1) cuboid island with three different $\sigma$.

Figure 4.15: Several snapshots in the evolution of an initial cuboid with dimension (3.2, 3.2, 0.1) towards its equilibrium. (a) $t = 0$; (b) $t = 0.0050$; (c) $t = 0.01$; (d) $t = 0.08$. The computational parameter is chosen as $\sigma = \cos(5\pi/6)$. 
4.3 Numerical results

Figure 4.16: Several snapshots in the evolution of the interface between the thin film and substrate towards the thin film’s equilibrium, and the initial cuboid is chosen with dimension $(3.2, 3.2, 0.1)$. The computational parameter is chosen as $\sigma = \cos(5\pi/6)$.

Figure 4.17: Several snapshots in the evolution of an initial cuboid with dimension $(6.4, 6.4, 0.1)$ until its pinch off. (a) $t = 0$; (b) $t = 0.005$; (c) $t = 0.010$; (d) $t = 0.031$. The computational parameter is chosen as $\sigma = \cos(5\pi/6)$. 
4.3 Numerical results

Figure 4.18: Several snapshots in the evolution of the cross section profile of the thin film along $y$-direction or diagonal direction until its pinch off, where the initial cuboid is chosen with dimension $(6.4, 6.4, 0.1)$. (a) $t = 0$; (b) $t = 0.005$; (c) $t = 0.010$; (d) $t = 0.031$. The computational parameter is chosen as $\sigma = \cos(5\pi/6)$.

and the parameter is chosen as $\sigma = \cos(5\pi/6)$. As shown in Fig. 4.15, the thin film evolves into a single spherical geometry. During the evolution, the corners retract much more slowly than the edges at the beginning, see Fig. 4.16. This phenomenon of corner accumulation has also been observed in experiment [117]. These corners at last catch up with the edges and the contact line moves towards a circular shape. If we enlarge the size of the thin film, as is depicted in Fig. 4.17, the thin film demonstrates the similar corner accumulation at the beginning but finally pinches off and forms hole in the centre, see Fig. 4.18. These two examples have also been numerically simulated in [66] via the phase field approach. Our numerical results are consistent with theirs.
4.3 Numerical results

4.3.5 Some special geometries

We investigate the morphology evolutions for islands initially given with some special geometries, such as the cross shape and square ring. Without special mention, the height of the initial thin film is always chosen to be 1, and the computational material constant is chosen as \( \sigma = \cos \frac{3\pi}{4} \).

As illustrated in Fig. 4.19, it demonstrates several stages of the geometry evolution of an initial cross-shaped island. The island is chosen with a cube attached with four equal limbs, and the four limbs are given by cuboids with dimension \((1, 4, 1)\). From the figure, we can observe that thin film eventually evolves into a single island with spherical geometry. However, if the four limbs are replaced with longer cuboids, the evolution could be quite different, see Fig. 4.20. As depicted in the figure, the four limbs are chosen with \((1, 6, 1)\) cuboid. Instead of forming a single island, the cross-shaped film undergoes pinch off at the joint and breaks up into five small islands. Fig. 4.21 and Fig. 4.22 are illustrations of the dynamic interface between the film and the substrate for the case of Fig. 4.19 and Fig. 4.20 respectively. It clearly demonstrates the migrations of the contact line during the evolution. When the thin film forms a single island, the contact line evolves into a circular shape. On the contrary, when pinch-off event happens, the contact line, which is a closed curve, breaks up into five closed curves simultaneously.

We next consider the case when the initial thin film is given as a square ring with wall thickness equaling 1 but different dimensions for the outer edges. We start by considering the evolution of a small square ring with the length of outer edges chosen as 2.5, see Fig. 4.23. As depicted in the figure, it clearly demonstrates the geometry evolution of the island as well as the cross-section profiles. The square ring firstly evolves into a ringlike shape but with different heights in different cross-section directions. However, as time evolves, the ring becomes a toroidal shape with same height in all cross-section orientations, see Fig. 4.23(c). At the same time, the toroidal film is also migrating towards its centre. If we enlarge the length of the outer edges for the initial thin film, the thin film will undergo pinch-off, see Fig. 4.24.
4.3 Numerical results

Figure 4.19: Several snapshots in the evolution of an initially cross-shaped island towards its equilibrium shape. Here the island consist of four (1,4,1) cuboids forming the limbs and one (1,1,1) cube in the centre, (a) $t = 0$; (b) $t = 0.15$; (c) $t = 0.5$; (d) $t = 0.9$; $\sigma = \cos(3\pi/4)$.

Figure 4.20: Several snapshots in the evolution of an initially cross-shaped island before its pinch-off. Here the island consist of four (1,6,1) cuboids forming the limbs and one (1,1,1) cube in the centre, (a) $t = 0$; (b) $t = 0.05$; (c) $t = 0.15$; (d) $t = 0.386$, $\sigma = \cos(3\pi/4)$. 
Figure 4.21: Several illustrations of the dynamic interface between the substrate and the island film (shaded in blue) for an initially cross-shaped island. The computational set up is as same as Fig. 4.19.

Figure 4.22: Several illustrations of the dynamic interface between the substrate and the island film (shaded in blue) for an initially cross-shaped island. The computational set up is as same as Fig. 4.20.
Figure 4.23: Several snapshots in the evolution of an initial island of square ring obtained from \((2.5, 2.5, 1)\) cuboid by cutting out a \((1.5, 1.5, 1)\) cuboid. (a) \(t = 0\); (b) \(t = 0.15\); (c) \(t = 1.0\); (d) \(t = 1.5\). The material constant is chosen as \(\sigma = \cos(3\pi/4)\).
4.3 Numerical results

Figure 4.24: Several snapshots in the evolution of an initial island of square ring obtained from a (3.5, 3.5, 1) cube by cutting out a (2.5, 2.5, 1) cube. (a) $t = 0$; (b) $t = 0.15$; (c) $t = 0.4$; (d) $t = 0.614$. The material constant is chosen as $\sigma = \cos(3\pi/4)$.

Figure 4.25: Several snapshots in the evolution an initial island of square ring obtained from a (5, 5, 1) cube by cutting out a (6, 6, 1) cube. (a) $t = 0$; (b) $t = 0.15$; (c) $t = 0.7$; (d) $t = 1.004$. The material constant is chosen as $\sigma = \cos(3\pi/4)$. 
and Fig. 4.25. The length of the outer edges could control the number of the islands the thin film breaks up into. As depicted in Fig. 4.24, it reveals the geometry evolution and the migrations of the two contact lines of the thin film for a square ring with the length of outer edges chosen as 3. As times evolves, the thickness of the film becomes various in different cross-section directions. The thick becomes even thicker and the thin becomes even thinner, thus making the thin film breaking up into 4 pieces finally. If the length of the outer edges for the initial square ring is further increased, then thin film is possible to break up into more small islands, see Fig. 4.25. This could be explained by Rayleigh instability [99]. For the cylinder, a small volume-preserving perturbation with wavelength exceeding the circumference of the cylinder could grow exponentially in order to reduce the surface area of the cylinder, thus the cylinder will break up into a series of small spherical islands. This breakup has been verified by our previous numerical examples, see Fig. 4.11 and Fig. 4.12. In addition to geometry of cylinder, the Rayleigh instability for more complex geometries such as torus has received great attention and has been studied theoretically and experimentally recently [85,88]. Analogous to the cylinder, a wavelength perturbation of torus in the azimuthal direction could also force the torus to break up into small particles. However, the existence of the axial curvature plus the periodicity in the azimuthal direction make the study much complicated. In the axial direction, the torus is unstable and will always migrate towards the centre to form spherical shape by decreasing the major radius and increasing minor radius. Experiments by E. Pairam [88] show that toroidal droplets can break up into a precise number of droplets or only shrink towards its centre to from a single spherical droplet, depending on the initial aspect ratio of the torus. This demonstrates that the Rayleigh instability in the azimuthal direction and shrinking instability in the axial direction are competing with each other to determine the dynamics geometries of the torus. Here for solid-thin film on a substrate, our numerical examples for square ring has clearly verified this theory.
4.4 Extension to weakly anisotropic case

In the previous section, we have proposed a variational formulation for the sharp interface model of solid-state dewetting with isotropic surface energy. Here we want to extend this variational form to the case when the surface energy is anisotropic. In isotropic case, the variation formulation for the chemical potential is given as

\[
\int_S \mu n \cdot g dS - \int_S \nabla_s X \cdot \nabla_s g dS = 0, \quad \forall g \in (H^1_0(S))^3. \tag{4.4.1}
\]

Given the chemical potential \( \mu = \nabla_s \cdot \xi \), for \( g \in (H^1_0(S))^3 \), a similar equation has been derived for anisotropic case [34, 94, 115], which reads as

\[
\int_S \mu n \cdot g dS - \int_S \gamma(n) \nabla_s X \cdot \nabla_s g dS = 3 \sum_{k,l=1}^3 \int_S \xi_k n_l \nabla_s x_k \cdot \nabla_s g_l dS. \tag{4.4.2}
\]

4.4.1 Variational formulation

Based on Eq. (4.4.2), the variational formulation for the sharp interface model Eqs. (3.4.5), (3.4.6), (3.4.8) and (3.4.9) can be stated as follows: given the initial surface \( S(0) = X(U, 0) \) with its boundary \( \Gamma(0) = X(\partial U, 0) \), we want to find \( X \in W^1_\Gamma(U), \mu \in H^1(S) \) such that

\[
\langle \partial_t X, \nu, \phi \rangle_S + \langle \nabla_s \mu, \nabla_s \phi \rangle_S = 0, \quad \forall \phi \in H^1(S), \tag{4.4.3a}
\]

\[
\langle \mu, n \cdot g \rangle_S - \langle \gamma(n) \nabla_s X, \nabla_s g \rangle_S = 3 \sum_{k,l=1}^3 \langle \xi_k n_l \nabla_s x_k \cdot \nabla_s g_l \rangle_S, \quad \forall g \in (H^1_0(S))^3, \tag{4.4.3b}
\]

with \( S = S(t) \). \( \Gamma = \Gamma(t) \) is determined via the following variational formulation: find \( \Gamma = X_t(\partial U, t), \kappa \in H^1(\Gamma) \) such that

\[
\langle \partial_t X_t, n_t, \varphi \rangle_\Gamma + \varepsilon^2 \langle M_t \partial_s \kappa, \partial_s \varphi \rangle_\Gamma = -\eta \langle c_\gamma^\top \cdot n_t - \sigma, \varphi \rangle_\Gamma, \quad \forall \varphi \in H^1(\Gamma), \tag{4.4.4a}
\]

\[
\langle \kappa, n_t \cdot \omega \rangle_\Gamma - \langle \partial_s X_t, \partial_s \omega \rangle_\Gamma = 0, \quad \forall \omega \in (H^1(\Gamma))^3. \tag{4.4.4b}
\]

Here the smooth regularization for the contact line migration is given as

\[
\partial_t X_t = \varepsilon^2 \partial_s (M_t \partial_s \kappa) n_t - \eta [c_\gamma^\top \cdot n_t - \sigma] n_t, \tag{4.4.5}
\]
where \( M_\Gamma = (c_\gamma \cdot n_r - \sigma)^2 \). As the contact line for the equilibrium shape is no longer a circle, we add this mobility \( M_\Gamma \) to ensure that when the numerical solution approaches the steady state, the contact line satisfies anisotropic Young equation

\[
\gamma(n_r) = \frac{c_\gamma \cdot n_r - \sigma}{\sqrt{M_\Gamma}} = 0.
\]

\[\text{(4.4.6)}\]

### 4.4.2 Full-discretization scheme

Given the spatial discretization and temporal discretization, the fully discrete parametric finite element method for solid-state dewetting with weakly anisotropic surfac energy can be stated as follows: assume \( S_0 = \bigcup_{j=1}^{N} \bar{D}_j \) is a discretization of the initial surface \( S(0) \) with good mesh quality, and \( \Gamma_0 = \bigcup_{j=1}^{N} \bar{h}_j \), for \( 1 \leq m \leq M - 1 \), we want to find \( S_{m+1} : X_{m+1} \in \mathcal{W}_h^{m+1}(S_m), \mu_{m+1} \in \mathcal{V}_h \), such that

\[
\begin{align*}
\langle X_{m+1} - X_m, \phi \rangle_{S_m} + \langle \nabla S X_{m+1}, \nabla \phi \rangle_{S_m} &= 0, \quad \forall \phi \in \mathcal{V}_h(S_m), \quad \text{(4.4.7a)} \\
\langle \mu_{m+1} - \gamma(n_m) \nabla S X_{m+1}, \nabla \phi \rangle_{S_m} &= \sum_{i,k=1}^{3} \langle \xi_i^m \nabla S x_i^m, n_i^m \nabla \phi \rangle_{S_m}, \quad \forall \phi \in \mathcal{V}_0(S_m)^3, \quad \text{(4.4.7b)}
\end{align*}
\]

where \( \Gamma_{m+1} \) is determined as follows: find \( \Gamma_{m+1} : X_{\Gamma_{m+1}} \in \mathcal{V}_h(\Gamma_m)^3, \kappa_{m+1} \in \mathcal{V}_h(\Gamma_m) \), such that

\[
\begin{align*}
\langle X_{\Gamma_{m+1}} - X_{\Gamma_m}, \varphi \rangle_{\Gamma_m} + \varepsilon^2 \langle M_{\Gamma_m} \partial_s \kappa_{m+1}, \varphi \rangle_{\Gamma_m} &= 0, \quad \forall \varphi \in \mathcal{V}_h(\Gamma_m), \quad \text{(4.4.8a)} \\
\langle \partial_s X_{\Gamma_{m+1}}, \partial_s \omega \rangle_{\Gamma_m} &= 0, \quad \forall \omega \in \mathcal{V}_h(\Gamma_m)^3. \quad \text{(4.4.8b)}
\end{align*}
\]

Here \( M_{\Gamma_m} = (c_\gamma^m \cdot n_{\Gamma_m} - \sigma)^2 \), \( \xi^m = (\xi_1^m, \xi_2^m, \xi_3^m) \), \( g_h = (g_{h,1}, g_{h,2}, g_{h,3}) \), \( X^m = (x_1^m, x_2^m, x_3^m) \). For the scheme, we have the following theorem,

**Theorem 4.4.1 (Well-posedness of the PFEM scheme).** The discrete variational problem, Eqs. (4.4.7a), (4.4.7b), (4.4.8a) and (4.4.8b) is well-posed.

**Proof.** The proof of this theorem is the same as proof of Theorem 4.2.1 by noting that \( \gamma(n_m) \) is always positive.

\[\square\]
In view of the definition of $\xi$ vector, one can defined: $\xi^m$ as

$$\xi^m_j = \xi^m \bigg|_{D^m_j} = \nabla \tilde{\gamma}_j (n^m_j). \quad (4.4.9)$$

In addition, $c^\gamma_\Gamma^m$ is defined as

$$c^\gamma_\Gamma^m_{m,j} = c^\gamma_\Gamma^m |_{h^m_j} = (\xi^m_{jk} \cdot n^m_{jk}) c^\Gamma^m_{m,j} - ((\xi^m_{jk} \cdot c^\Gamma^m_{m,j}) n^m_{jk}) \quad (4.4.10)$$

with $D^m_{jk}$ contains the line segment $h^m_j$. 

For the weakly anisotropic surface energy, if $\gamma(n)$ is chosen as the cubic surface energy defined in Eq. (1.1.6) with $a$ smaller enough, the mesh equality can be well preserved like the isotropic case. However, when the surface energy is chosen as the cusps or facet surface energies defined in Eq. (2.5.2), the mesh quality will deteriorate along the time evolution, thus mesh regularization is necessary in order to make the scheme stable. We refer to [6] for the volume-preserving mesh regularization method.

### 4.4.3 Numerical results

In this section, we report some numerical simulation results under the anisotropic surface energies. We will mainly consider the following cubic anisotropy

$$\gamma_c(n) = 1 + a[n_1^4 + n_2^4 + n_3^4], \quad 0 \leq a < \frac{1}{3}. \quad (4.4.11)$$

Fig. 4.26 shows the convergence results of the equilibrium shapes with $\sigma = \cos\left(\frac{15\pi}{36}\right), a = 0.25$. We compute the equilibrium shapes for an initial $(1, 2, 1)$ cuboid with different meshes, which are given with a set of small isosceles right triangles. If we define the mesh size indicator $h$ as the length of the hypotenuse of the right triangle, then Mesh1 represents the initial mesh with $h = h_0 = 0.125$, and the time step is chosen as $\tau = \tau_0 = 0.00125$ for computation. Meanwhile, the time step for Mesh2 and Mesh3 are chosen as $\tau = \frac{\tau_0}{4}$ and $\tau = \frac{\tau_0}{16}$ respectively. For easy comparison, we have depicted the $x$-directional cross-section profiles both for the numerical equilibrium shapes and the theoretical equilibrium shape. We can clearly observe that as the mesh size decrease, the numerical cross-section profiles
are convergent to the cross-section profiles of the theoretical equilibrium shapes. This prove that our PFEM scheme for the weakly anisotropic surface energy is convergent.

![Figure 4.26](image)

Figure 4.26: Comparison of the cross section profiles of the numerical equilibrium with the theoretical equilibrium shape obtained from Winterbottom construction. The material constant is given as $\sigma = \cos \frac{15\pi}{36}$.

![Figure 4.27](image)

Figure 4.27: Several snapshots in the evolution of an initial $(1, 2, 1)$ cuboid towards its equilibrium under the cubic anisotropy with $a = 0.25$. The material constant is chosen as $\sigma = \cos \frac{5\pi}{6}$. 
Fig. 4.27 shows the geometry evolution of an island film under the cubic anisotropy with $a = 0.25$. The initial island is a cuboid with dimension $(1, 2, 1)$, and the material constant is chosen as $\sigma = \cos(\frac{5\pi}{6})$. The island film evolves towards a shape with corners. In order to investigate the effect of the degree of anisotropy on the equilibrium shape, we have shown the equilibrium shapes under different $a$ with same $\sigma = \cos \frac{5\pi}{6}$. As clearly observed from Fig. 4.28(a)-(c), the corners of the equilibrium shapes become sharper as $a$ becomes bigger, which is consistent with the theoretical predications. On the other hand, we compute the equilibrium shape by fixing the degree of the anisotropy $a = 0.25$, and changing the material constant $\sigma$. The equilibrium shapes for $\sigma = 0.5, 0, -0.5$ are given in Fig. 4.29(a),(b) and (c) respectively. In addition, the corresponding cross-section profiles and contact lines of the equilibrium shapes are also shown in Fig. 4.30. From these figures, we can clearly see that $\sigma$ determines the contact angles of the equilibrium shape.

Unlike the isotropic case, a rotation of the surface energy density is equivalent to a rotation of the corresponding equilibrium shape. Assume $M_x(\theta)$ is a rotation matrix, which represents an anti-clockwise rotation about the x-axis in three dimensions under the right-hand rule. To observe the rotation effects, we compute the equilibrium shapes under the anisotropies $\gamma = \gamma_c(M_x(\frac{\pi}{6}n))$ and $\gamma = \gamma_c(M_x(-\frac{\pi}{6}n))$. As shown in Fig. 4.31, the equilibrium shapes exhibit the corresponding rotation effects.
4.4 Extension to weakly anisotropic case

Figure 4.29: The equilibrium shapes of an initial \((1, 2, 1)\) cuboid under cubic anisotropy with \(a = 0.25\). (a) \(\sigma = 0.5\); (b) \(\sigma = 0\); (c) \(\sigma = -0.5\).

Figure 4.30: (a) The cross-section profiles of the equilibrium shapes. (b) The contact lines of the equilibrium shapes.
along $x$-axis. In addition to the cubic anisotropy, we have also performed numeri-

cal simulations for the ellipsoidal anisotropy defined in Eq. (1.1.7). Fig. 4.32 shows

![Figure 4.31](image1.png)

Figure 4.31: The equilibrium shapes of an initial $(1, 2, 1)$ cuboid, and the material constant is chosen as $\sigma = \cos \frac{3\pi}{4}$. (a) $\gamma = \gamma_c(M_x(\frac{\pi}{6})n); (b) \gamma = \gamma_c(M_x(-\frac{\pi}{6})n)$.

![Figure 4.32](image2.png)

Figure 4.32: Several snapshots in the evolution of an initial $(1, 2, 1)$ cuboid towards its equilibrium under the ellipsoidal anisotropy with $a_1 = 2, a_2 = 1, a_3 = 1$. The material constant is chosen as $\sigma = \cos \frac{3\pi}{4}$. (a) $t = 0$; (b) $t = 0.02$; (c) $t = 0.04$; (d) $t = 1.0$. 

4.4 Extension to weakly anisotropic case
the geometry evolution of an initially cuboid island towards its equilibrium shape with \( \sigma = \cos \frac{3\pi}{4} \). The surface energy density is chosen as \( \gamma(n) = \sqrt{2n_1^2 + n_2^2 + n_3^2} \).

From the figure, we can see that thin film eventually obtains the equilibrium with ellipsoidal geometry. This is consistent with our predictions since the corresponding Wulff shape for the anisotropy \( \gamma(n) = \sqrt{2n_1^2 + n_2^2 + n_3^2} \) is given by an ellipsoid with implicit equation \( \frac{x^2}{2} + y^2 + z^2 = 1 \).
Extensions

In this chapter, we mainly focus on some extensions of the sharp interface model. We will extend the model to the strongly anisotropic case and curved substrate. Moreover, the migration of the toroidal thin film on the flat substrate will be investigated under the assumption of axis-symmetry.

5.1 For strongly anisotropic surface energy

In 2D, some orientations are missing in the equilibrium shape (see Fig. 5.1(a)) when the surface stiffness $\gamma(\theta) + \gamma''(\theta)$ is negative for some orientations [67,105]. In this strongly anisotropic case, the anisotropic surface diffusion flow becomes backward and ill-posed. In order to avoid this ill-posedness, the Willmore energy regularization is generally utilized [30,58]. In 3D, a similar regularization is necessary when missing orientations appear in the equilibrium shape (see Fig. 5.1(b)). Therefore in this section, we perform the extension in 3D and derive the model for strongly anisotropic case.
Figure 5.1: Ears appear in $\xi$-plot for strongly anisotropic surface energy. (a) $\gamma(\theta) = 1 + 0.2\cos(4\theta)$ in 2D; (b) $\gamma(\mathbf{n}) = 1 + (n_1^4 + n_2^4 + n_3^4)$ in 3D.

5.1.1 The regularized energy and first variation

The Willmore energy can be written as

$$W_r = \int \int_S H^2 \, dS.$$  \hfill (5.1.1)

We have the following lemmas which is helpful for calculating the first variation of the Willmore energy functional.

**Lemma 5.1.1.** Assume $S \in \mathbb{R}^3$ is a $C^k$-hypersurface, with $k \geq 3$. $H$ is the mean curvature of $S$, then the normal derivative of $H$ is given by

$$\partial_n H = -(\kappa_1^2 + \kappa_2^2) = -(H^2 - 2K),$$ \hfill (5.1.2)

where $\kappa_1, \kappa_2$ are the two principle curvatures of the surface, $K$ is the Gauss curvature.

**Proof.** We omit the proof as this is a simple application of the signed distance function defined in Eq. (3.1.42) and the proof can be found in [58,64]
5.1 For strongly anisotropic surface energy

Lemma 5.1.2. Let $S \in \mathbb{R}^3$ be a $C^k$-hypersurface with smooth boundary, and $k \geq 4$. If $W_r(S) = \iint_S \mathcal{H}^2 \, dS$, then we have the first variation of $J(S)$ in the direction of $V$ is given by

$$dW_r(S; V) = 2 \int_{\Gamma} [\nabla_s \mathcal{H} \cdot c_r](n \cdot V_0) \, d\Gamma - \int_{S} \mathcal{H}^2 c_r \cdot V_0 \, dS. \quad (5.1.3)$$

Here $\mathcal{K}$ is the Gaussian curvature.

Proof. To calculate the variation, using Eqs. (3.1.41) and (3.1.44), we have

$$dW_r(S; V) = \iint_S 2\mathcal{H}(-\Delta_s (n \cdot V_0)) \, dS + \iint_S [\partial_n \mathcal{H}^2 + \mathcal{H}^3] n \cdot V_0 \, dS + \int_{\Gamma} \mathcal{H}^2 V_0 \cdot c_r \, d\Gamma. \quad (5.1.4)$$

Not that $\partial_n \mathcal{H} = -(\mathcal{H}^2 - 2\mathcal{K})$ by lemma. 5.1.1, integration by parts based on Eq. (3.1.10), we get

$$dW_r(S; V) = 2 \int_{\Gamma} [\nabla_s \mathcal{H} \cdot c_r](n \cdot V_0) \, d\Gamma - 2 \int_{S} [\Delta_s \mathcal{H} + \mathcal{H}^3] n \cdot V_0 \, dS + \int_{\Gamma} \mathcal{H}^2 V_0 \cdot c_r \, d\Gamma. \quad (5.1.5)$$

The total dimensionless surface energy after regularization becomes

$$W_{r, \text{reg}} = W + \frac{\delta^2}{2} W_r = \iint_S \gamma(n) \, dS - \sigma A(\Gamma) + \frac{\delta^2}{2} \iint_S \mathcal{H}^2 \, dS. \quad (5.1.6)$$

From the lemma. 5.1.2 and the variation of $W$, also noting that on the boundary,

$$n \cdot V_0 = (P_{sw} n) \cdot V_0 = (n \cdot n_r)(n_r \cdot V_0), \quad (5.1.7)$$
we can easily obtain that
\[
dW^{\delta}_{\text{reg}}(S; \mathbf{V}) = \int_S \left[ \nabla_S \cdot \xi - \delta^2 (\Delta_s \mathcal{H} + \frac{\mathcal{H}^3}{2} - 2\mathcal{H} \mathcal{K}) \right] V_0 \cdot n \ dS \\
+ \int_{\Gamma} \left[ c^\gamma_{1r} \cdot n_r - \sigma + \delta^2 (\nabla_S \cdot c_r)(n \cdot n_r) \right] V_0 \cdot n_r \ d\Gamma \\
+ \delta^2 \int_{\Gamma} \left[ \mathcal{H}^2 c_r \cdot \nabla_S (n \cdot V_0) \right] dS.
\]
(5.1.8)

The variation of the total energy with respect to the surface \( S \) is immediately given by
\[
\frac{\delta W^{\delta}_{\text{reg}}}{\delta S} = \nabla_s \cdot \xi - \delta^2 (\Delta_s \mathcal{H} + \frac{\mathcal{H}^3}{2} - 2\mathcal{H} \mathcal{K}).
\]
(5.1.9)

Since a higher order energy is added to the surface energy for regularization, the governing equations will result in a sixth order geometric PDE, thus an additional boundary condition should be included for them. In consideration of the undesirable term in the variation \( \mathcal{H} c_r \cdot \nabla_S (n \cdot V_0) \), if we want to obtain the variation of \( W^{\delta}_{\text{reg}} \) with respect to the boundary \( \Gamma \), we need to impose the following zero curvature boundary condition
\[
\mathcal{H} \bigg|_{\Gamma} = 0.
\]
(5.1.10)

Such boundary condition is also imposed in two dimensions, which serves as the condition to make sure the system is dissipative. Therefore the variation of \( W^{\delta}_{\text{reg}} \) with respect to the \( \Gamma \) is
\[
\frac{\delta W^{\delta}_{\text{reg}}}{\delta \Gamma} = c^\gamma_{1r} \cdot n_r - \sigma + \delta^2 (\nabla_S \cdot c_r)(n \cdot n_r).
\]
(5.1.11)

5.1.2 The regularized model

Similar to the weakly anisotropic case, the variation of the total energy with respect to the surface \( S \) and \( \Gamma \) give the chemical potential and contact line migration velocity, respectively. Now we assume \( S \) is a \( C^k \)-hypersurface with smooth boundary, where \( k \geq 6 \). Let \( \mathbf{X} \) and \( \mathbf{X}_r \) denote a local parametrization of \( S \) and \( \Gamma \) respectively.
5.2 For curved substrate

The sharp interface model for solid-state dewetting with strongly anisotropic surface energy is given by

\[
\partial_t X = \Delta_s \mu n, \quad t > 0, \tag{5.1.12}
\]

\[
\mu = \nabla_s \cdot \xi - \delta^2(\Delta_s H + \frac{H^2}{2} - 2HK), \tag{5.1.13}
\]

\[
H = -\Delta_s X \cdot n, \quad K = \frac{H^2 + \Delta_s n \cdot n}{2}, \tag{5.1.14}
\]

together with the following boundary conditions

(1) contact line condition

\[
\Gamma \subset S_{\text{sub}}, \quad t \geq 0, \tag{5.1.15}
\]

(2) relaxed contact angle condition

\[
\partial_t X_\Gamma = -\eta \left[ c_r^1 \cdot n_r - \sigma + \delta^2(\nabla_s H \cdot c_r)(n \cdot n_r) \right] n_\Gamma, \quad t \geq 0; \tag{5.1.16}
\]

where \( c_r^1 = (\xi \cdot n) c_r - (\xi \cdot c_r) n, \ n_r = \frac{1}{\sqrt{n_1^2 + n_2^2}}(n_1, n_2, 0), \ \sigma = \frac{\gamma_{VS} - \gamma_{FS}}{\gamma_0}. \)

(3) zero-mass flux condition

\[
c_r \cdot \nabla_s \mu \bigg|_\Gamma = 0, \quad t \geq 0; \tag{5.1.17}
\]

(4) zero-curvature condition

\[
H \bigg|_\Gamma = 0, \quad t \geq 0. \tag{5.1.18}
\]

The mass conservation and energy dissipation can also be proved easily. Here we omit the proof as it is similar to that for weakly anisotropic case.

5.2 For curved substrate

Previously we always assume that the rigid substrate is flat and represented by the \( xOy \) plane, however, experiments have shown that the topologies of the substrate
could have great influence on dewetting of the thin films. For example, templated dewetting shows that substrate in order pattern could produce thin films of ordered structure. Thus it is necessary to extend our sharp interface model to the curved substrate case. See Fig. 5.2, $S$ is the open surface representing the interface between the vapor and film while $S_{\text{sub}}$ is the surface representing the substrate. $\Gamma \subset \text{Su}$ is a space curve in three dimensions, which represents on the contact line of the substrate and the film. $n$ is the outer unit normal vector of $S$ and $n_{\text{sub}}$ is the outer unit normal vector of the substrate $S_{\text{sub}}$. $n_{\Gamma}$ is the outer unit normal vector of the contact line $\Gamma$ in $S_{\text{sub}}$. From the above defintion, we can clearly see the following equations hold

\begin{align}
  n_{\Gamma}(x) & \perp \tau_{\Gamma}(x), \quad n_{\Gamma}(x) \perp n_{\text{sub}}(x), \quad \forall x \in \Gamma, \\
  c_{\Gamma}(x) & \perp \tau_{\Gamma}(x), \quad c_{\Gamma} \perp n(x), \quad \forall x \in \Gamma.
\end{align}

If we assume that the $\gamma_{FS}, \gamma_{VS}$ are constants and $\gamma_{FV} = \gamma(n)$, then we the total dimensionless surface energy can be written as

\begin{equation}
  W = W_{\text{int}} + W_{\text{sub}} = \int_S \gamma(n) \, dS - \sigma A(\Gamma, S_{\text{sub}}),
\end{equation}

Figure 5.2: A schematic illustration of solid-state dewetting on a curved substrate.
where $\sigma = \frac{\gamma_V - \gamma_S}{\gamma_0}, \ A(\Gamma; S_{sub})$ is the area enclosed by the space curve $\Gamma$ on the surface $S_{sub}$.

Here we assume the substrate is not deformable, thus surface $S_{sub}$ is a fixed surface. Give the surface $S$ as the initial surface with boundary $\Gamma \subset S_{sub}$, consider a transformation $T_\varepsilon$ of $S$. Under this transformation, we always assume that the boundary of $S$ is attached on the surface $S_{sub}$, that is

$$T_\varepsilon \Gamma \subset S_{sub}. \tag{5.2.3}$$

The first variation of $W_{int}$ in the direction of $V$ is given by Eq. (3.2.3),

$$dW_{int}(S; V) = \int \int_S \nabla_s : \xi \ dS + \int _\Gamma (c_r^\gamma \cdot V_0) \ d\Gamma. \tag{5.2.4}$$

For the second part, if we assume that the surface of $S_{sub}$ enclosed by $\Gamma$ is given by $S_\Gamma$. Consider the transformation on $S_\Gamma$, such that

$$T_\varepsilon S_\Gamma = S_\Gamma^\varepsilon, \quad T_\varepsilon \Gamma = \Gamma^\varepsilon \subset S_{sub}. \tag{5.2.5}$$

This indicates that the transformation $T_\varepsilon$ satisfies the following on the boundary of $S_\Gamma$

$$V \parallel T_\varepsilon S_{sub}, \quad V \perp n_{sub}. \tag{5.2.6}$$

For $W_{sub}(\Gamma) = \int \int_{S_\Gamma} dS_\Gamma$, by using Eq. (3.2.6) again, we obtain

$$dW_{sub}(\Gamma; V) = -\sigma \int _\Gamma (n_r \cdot V_0) \ dS. \tag{5.2.7}$$

Similarly, we know that $V_0 |_{\Gamma} \perp n_{sub}$, thus we can project $c_r^\gamma$ on the tangential space of $S_{sub}$, we obtain

$$dW_{int}(S; V) = \int \int_S \nabla_s : \xi \ dS + \int _\Gamma (c_r^\gamma \cdot n_r)(n_r \cdot V_0) \ d\Gamma. \tag{5.2.8}$$

Thus combine the variation of $W_{int}$ and $W_{sub}$, we can get the variation is exactly the same as Eq. (3.2.6). This indicates that the sharp interface model for solid-state dewetting on a curved substrate is consistent to the the models for solid-state
dewetting on a flat substrate. For curved substrate, the contact line migrates along the substrate in the directions \( \mathbf{n}_r \). Thus if we denote the \( \mathbf{X} \) and \( \mathbf{X}_r \) as the local parameterization of \( S \) and \( \Gamma \) respectively. Then the dimensionless sharp interface model for solid-state dewetting on a curved substrate is given by

\[
\partial_t \mathbf{X} = \Delta S \mu \mathbf{n}, \quad t > 0, \tag{5.2.9}
\]

\[
\mu = \nabla_S \cdot \xi, \quad \xi = \nabla \tilde{\gamma}(\mathbf{n}), \tag{5.2.10}
\]

together with the following boundary conditions

1. **contact line condition**

   \[
   \Gamma \subset S_{\text{sub}}, \quad t \geq 0, \tag{5.2.11}
   \]

2. **relaxed contact angle condition**

   \[
   \partial_t \mathbf{X}_r = -\eta \left[ \mathbf{c}_r \cdot \mathbf{n}_r - \sigma \right] \mathbf{n}_r, \quad t \geq 0, \tag{5.2.12}
   \]

   where \( \mathbf{c}_r = (\xi \cdot \mathbf{n}) \mathbf{c}_r - (\xi \cdot \mathbf{c}_r) \mathbf{n}, \quad \mathbf{n}_r = \frac{\tau_r \times \mathbf{n}_{\text{sub}}}{|\tau_r \times \mathbf{n}_{\text{sub}}|}, \quad \sigma = \frac{\gamma_{\text{VS}} - \gamma_{FS}}{\gamma_0}, \)

3. **zero-mass flux condition**

   \[
   (\mathbf{c}_r \cdot \nabla_S \mu)_{\Gamma} = 0, \quad t \geq 0. \tag{5.2.13}
   \]

### 5.3 For axis-symmetric case

In last chapter, numerical simulations for the square ring demonstrate that when the inner hole is not large enough, the hollow can form a toroidal shape and then migrate towards the centre. Thus here we want to study this migration mechanism in the form of axis-symmetry.

#### 5.3.1 The sharp interface model

The interface between the vapor and thin film is denoted by surface

\[
S = (r(s) \cos \varphi, r(s) \sin \varphi, z(s)) \tag{5.3.1}
\]
5.3 For axis-symmetric case

Figure 5.3: A schematic illustration of the solid-state dewetting, (a) an toroidal thin film on a flat substrate. (b) The cross-section profile (Γ₀) of an axis-symmetric thin film in a cylindrical coordinate system (r,z), with rᵢ, rₒ corresponding to the inner and outer contact line respectively.

Here r(s) is the radial distance, φ is the azimuth angle, z(s) is the film height. Then the total surface energy can be described as

\[ W = \int \int_S \gamma_{\text{FW}} \, dS + (\gamma_{\text{FS}} - \gamma_{\text{VS}}) \pi (r_o^2 - r_i^2) \].

(5.3.2)

\[ \gamma_{\text{FW}}, \gamma_{\text{FS}} \text{ and } \gamma_{\text{VS}} \text{ are constants and represent the surface energy densities of film/vapor, film/substrate and vapor/substrate respectively. } \]

\[ r_o, r_i \text{ are marked in Fig. 5.3, which are the radius of the outer and inner contact lines respectively.} \]

Denote \( \Gamma = X_a(s,t) = (r(s,t), z(s,t)) \), with \( 0 \leq s \leq L(t) \) and \( r(0,t) = r_i, r(L,t) = r_o \). If the length and surface energy density are scaled by L and γ₀ respectively, and the time scale is chosen as \( \frac{L^4}{B\gamma_0} \) with \( B = \frac{D_\gamma \gamma_0 \Delta \Omega}{k_B T_e} \), the contact line mobility is scaled by \( \frac{B}{L^3} \), then the dimensionless sharp interface model for solid-state dewetting in three dimensions with cylindrical symmetry can be stated as

\[ \partial_t X_a = \frac{1}{r} \partial_s (r \partial_s \mu) \, n_a, \quad (5.3.3) \]

\[ \mu = H = \kappa + \frac{\partial_s z}{r}, \quad (5.3.4) \]

together with the following boundary conditions;

(i) contact line condition

\[ z(0,t) = 0, \quad z(L,t) = 0, \quad (5.3.5) \]
For axis-symmetric case

(ii) relaxed (or dissipative) contact angle condition

\[
\frac{dr_i}{dt} = \eta (\cos \theta^i_c - \cos \theta_i), \quad \frac{dr_o}{dt} = -\eta (\cos \theta^o_c - \cos \theta_i), \quad (5.3.6)
\]

(iii) zero-mass flux condition

\[
\partial_s \mu(0, t) = 0, \quad \partial_s \mu(L, t) = 0; \quad (5.3.7)
\]

where \( \theta^i_c, \theta^o_c \) are the (dynamic) contact angles for the inner contact line and outer contact line, respectively, \( 0 < \eta < \infty \) denotes the dimensionless contact line mobility, and \( \theta_i \) is the isotropic Young’s angle with Young’s equation defined as

\[
\gamma_{FY} \cos \theta_i = \gamma_{VS} - \gamma_{FS}. \quad (5.3.8)
\]

The zero-mass flux condition is to ensure that the total volume of the thin film is conserved. A parametric finite element method can be applied to solve the sharp interface model with the initial thin film chosen as a tinny toroidal thin film. The contact line mobility is chosen big enough such that it will not drag the motion of the contact line.

5.3.2 A reduced model via Onsager’s principle

Figure 5.4: A schematic illusion of tiny toroidal tin film migration by decreasing \( R \) and increasing \( a \).

Numerical simulation demonstrates that the tiny toroidal thin film tends to migrate toward the centre in a constant speed while maintaining the two dimension
For axis-symmetric case

The equilibrium shape in the axial direction. The speed is inversely proportional to the total volume of the tin film. This good prosperity the torus preserve during the migration give as some motivations to reduce the complicated sharp interface model. Given the initial volume of the thin film as $M_0$, we now assume that the shape of the thin film in the axis direction is given as

$$
\begin{align*}
  r(\theta, t) &= R(t) + a(t) \sin \theta, \\
  z(\theta, t) &= a(t)(\cos \theta - \cos \theta_i),
\end{align*}
$$

(5.3.9)

The thin film migrates towards centre and preserve the total volume, so we have

$$M(t) \equiv A_0 = \pi R a^2 (2\theta_i - \sin(2\theta_i)).$$

(5.3.10)

The total surface energy can be obtained from (5.3.2)

$$W(t) = 2\pi R a(2\theta_i - \sin(2\theta_i)).$$

(5.3.11)

Substituting $a(t)$ by $M_0$ and $R(t)$ in $W(t)$, then taking derivative of $W(t)$ with respect to $t$, we obtain $\dot{W}(t)$

$$\dot{W} = \sqrt{\pi A_0 (2\theta_i - \sin(2\theta_i))} R^{-\frac{1}{2}} \dot{R}.$$  

(5.3.12)

On the other hand, by noting the unit normal vector $\mathbf{n}_a = (\sin \theta, \cos \theta)$, the normal velocity $v_n$ of the surface can be expressed as following,

$$v_n(\theta) = \dot{R} \sin \theta + \dot{a}(1 - \cos \theta_i \cos \theta).$$

(5.3.13)

The flux only has component in the axial tangential direction. If we set $\mathbf{\tau}$ as the unit vector in the tangential direction of the axial curve, we have

$$\nabla_s \cdot (J \mathbf{\tau}) = \frac{\partial_s (r J)}{J} = v_n(\theta),$$

(5.3.14)

this give the flux

$$J(\theta) \approx (\cos \theta_i - \cos \theta) a \dot{R}.$$  

(5.3.15)
5.3 For axis-symmetric case

Denote $\delta = a/R$, as $\delta \ll 1$, by Onsager’s principle, we have

$$J(\theta) = \frac{1}{R + a \sin \theta} \int_{-\theta_i}^{\theta} (R + a \sin \beta) v_n(\beta) a \, d\beta. \quad (5.3.16)$$

By $\pi Ra^2(2\theta_i - \sin(2\theta_i)) \equiv M_0$, take derivative with respect to $t$, we have

$$a \dot{R} = -2Ra. \quad (5.3.17)$$

Substituting above equation into Eq. (5.3.16), we obtain

$$J(\theta) = \frac{a}{R + a \sin \theta} [R \dot{R} \int_{-\theta_i}^{\theta} \sin \beta d\beta + aR \int_{-\theta_i}^{\theta} \sin^2 \beta d\beta + R \dot{a} \int_{-\theta_i}^{\theta} (1 - \cos \theta_i \cos \beta) d\beta + a \dot{a} \int_{-\theta_i}^{\theta} \sin \beta (1 - \cos \theta_i \cos \beta) d\beta]. \quad (5.3.18)$$

After a simple reduction, we have

$$J(\theta) = (\cos \theta_i - \cos \theta) \dot{R}a \left[ \frac{2 + \delta \sin \theta}{2 + 2\delta \sin \theta} + O(\delta^2) \right]$$

$$= (\cos \theta_i - \cos \theta) \dot{R}a \left[ 1 - \frac{1}{2} \delta \sin \theta + O(\delta^2) \right]. \quad (5.3.19)$$

So substituting the flux into the following surface integral, we have

$$\dot{W} = -\int_S J^2 \, dS = -2\pi a \int_{-\theta_i}^{\theta_i} (R + a \sin \theta) J(\theta)^2 \, d\theta$$

$$= -2\pi Ra^3 \dot{R}^2 g(\theta_i) + O(\delta^2), \quad (5.3.20)$$

with $g(\theta) = \theta(2 + \cos(2\theta)) - \frac{3}{2} \sin(2\theta)$. Combined Eq. (5.3.12) and Eq. (5.3.20), and noting the Eq. (5.3.10) thus we obtain the predicted migration rate $v$

$$v = -\dot{R}(t) \approx \frac{C(2\theta_i)}{M_0}, \quad (5.3.21)$$

where

$$C(\theta) = \frac{\pi(\theta - \sin \theta)^2}{(\theta(2 + \cos \theta)) - 3 \sin \theta}. \quad (5.3.22)$$

This means the migration rate depends on the initial volume of the thin film and the isotropic Young’s angle $\theta_i$. It is inversely proportionally to the volume with coefficient $C(2\theta_i)$. Thus we can obtain the dynamics of $R(t)$

$$R(t) = R_0 - \frac{C(2\theta_i)}{M_0} t, \quad 0 \leq t < t_d < \frac{R_0 M_0}{C(2\theta_i)}. \quad (5.3.23)$$
Fig. 5.5 shows the numerical results for the temporal evolution of the major radius $R(t)$ of the toroidal tin film as well as the theoretical formulation of $R(t)$ in Eq. (5.3.23). The isotropic Young’s angle $\theta_i$ is chosen as $\pi/2$, and the initial thin film is taken as the upper half of a torus with $R_0 = 4.0, a_0 = 0.5$. From the figure, we can see that the numerical points for $R(t)$ agree quite well with the analytical line from the beginning to the time $t_\delta$. As $a/R$ is small enough, the thin film is migrating towards its centre in a quasi-static state, and the cross section profile of the thin film is almost the two dimension equilibrium shape. Since $a/R$ is increasing as time evolves, the cross section profile will deteriorate and the approximation also becomes worse. So this explains that why there exist a critical time region that when the thin film is almost touch the centre, the reduced model is not applicable any more.

Fig. 5.6 shows that the migration rate of the thin film is inversely proportional to the initial volume of the thin film. The isotropic Young’s angle is chosen as $\theta_i = \pi/2$. From the figure, we can observe the numerical migration rate is indeed
inversely proportional to the initial volume and also it has a good agreement with the analytical result.

Fig. 5.7 shows the comparison of numerical coefficient \( C_h(2\theta_i) \) from the sharp interface model with the theoretical formulation of \( C(2\theta_i) \), see Eq. (5.3.22). The migration rate of the thin film is inversely proportional to the total volume and the coefficients depends on the isotropic Young’s angle \( \theta_i \). Where when \( \theta_i = \frac{\pi}{2} \), the coefficient reach maximum. This indicates that the contact line tends to hinder this migration.

![Graph showing comparison of migration speed](image)

**Figure 5.6:** Comparison of the numerical migration speed \( v \) obtained numerically from the sharp interface model (circles, squares or triangles) and the theoretical migration speed \( v \) by Eq. (5.3.21) (solid line).
5.3 For axis-symmetric case

Figure 5.7: Comparison of the numerical coefficient $C_h(2\theta_i)$ obtained numerically from the sharp interface model (blue circles) with the theoretical formulation of $C(2\theta_i)$ in Eq. (5.3.22).
Conclusion and Future Works

This thesis focuses on the derivation of sharp interface models for solid-state dewetting problem and development of efficient numerical approximations for solving the governing geometric partial differential equations. The problem has been studied both in two dimensions and three dimensions in the form of Cahn-Hoffman $\xi$-vector.

In chapter 2, the two-dimensional problem was studied via the energy variational approach. The equations for the equilibrium shape and its stability conditions were derived by calculating the first and second variation of the energy functional. We have presented the sharp interface model for solid-state dewetting in the form of Cahn-Hoffman $\xi$-vector. Moreover, a semi-implicit parametric finite element method was proposed for solving the sharp interface models. The mass conservation and energy dissipation were proved to be satisfied for the variational formulation and semi-discrete scheme. The strongly anisotropic case was also included via Willmore energy regularization. A similar parametric finite element method was presented. Numerical simulations for the evolution of small islands, large islands have demonstrated the accuracy of the model, efficiency of the numerical schemes and anisotropic effect on the island evolution. The power law for the edge retraction of semi-infinite thin film was investigated under the cusp surface energy.

In chapter 3, based on thermodynamic variation, we derived a sharp interface model for solid-state dewetting with anisotropic surface energy in three dimensions.
Unlike two dimensions, we calculate the energy variation by using the shape derivatives and speed method. The mass conservation and energy dissipation for the model were presented afterwards. In chapter 4, based on the model we presented a parametric finite element method for solving the sharp interface model with isotropic surface energy. The surface diffusion flow for the open surface can be approximated by a simple extension of variational formulation in two dimensions. The contact line migration for the plane curve was formulated with a small surface diffusion regularization. The parametric finite element scheme has also been extended to the weakly anisotropic case. Moreover, extensive numerical simulation results have validated the convergence of the discrete schemes, shown consistent morphological evolutions observed in physical experiments, and proven the accuracy of the models.

In Chapter 5, based on thermodynamic variation, the sharp interface model has been generalized to the case when the surface energy is strongly anisotropic and when the substrate is curved. Moreover, we studied the migration of toroidal thin film for solid-state dewetting under the cylindrical symmetry. We obtained a reduced model via Onsager’s Principle for describing the migration rate. This reduced model was then validated by numerical results.

Some future works can be summarised as follows.

- The parametric finite element method will be extended to the cases when the surface energy is strongly anisotropic and when the substrate is curved. However, this extension is not straightforward for the two cases. The introduction of the Gauss curvature in the governing equations for the strongly anisotropic case may require some techniques for a good variational formulation. In addition, when the substrate is curved, the contact line where the thin film, vapor and substrate meet becomes a space curve in three dimensions. The variational formulation as well as the smooth regularization for the plane curve will be extended for space curve.

- Although our parametric finite element scheme has some good properties with respect to the mesh distribution. However, this is only true for isotropic case.
For strongly anisotropic case, the polygonal mesh has high possibility to deteriorate. Therefore, a good mesh regularization is required to ensure the stability of the discrete scheme. Moreover, our mesh generation procedure is only applicable to an initially cuboid island, and efficient mesh generation algorithms for complex geometries need to be developed.

- Although there are some numerical convergence tests for parametric finite element method in solving surface diffusion flow [20], however, to our knowledge, the rigorous mathematical analysis for the convergence rate of PFEM scheme is still unclear. For solid-state dewetting problem, the complicated boundary conditions could further make the mathematical analysis more difficult.

- Our simulation examples will be set up more realistically in the further. This includes the simulations of hole growth, the power law for edge retraction. As a consequence, the computational cost as well as the storage could be very large. If possible, the parallel computation will be considered.

- The phase field approach to solid-state dewetting will be considered in the future as a comparison with the sharp interface approach. The sharp interface limit will be analysed. The numerical simulation results for the phase field approach and sharp interface approach could provide a benchmark for solid-state dewetting.

- The solid-state dewetting problem will be studied by including the elasticity of the materials, considering a deformable substrate and so on.
Taylor expansions for linear perturbation

Under the perturbation

\[ \mathbf{X}(\rho, \varepsilon) = \mathbf{X}(\rho, 0) + \varepsilon \mathbf{X}^1(\rho), \]  

(A.1)

we have

\[ \mathbf{V}_0 \equiv \partial_\varepsilon \mathbf{X}(\rho, \varepsilon) = \partial_\varepsilon \mathbf{X}(\rho, \varepsilon) \bigg|_{\varepsilon=0} = \mathbf{X}^1(\rho), \quad \partial_\varepsilon^2 \mathbf{X}(\rho, \varepsilon) = 0. \]  

(A.2)

We show the expansions of \( |\partial_\rho \mathbf{X}(\rho, \varepsilon)| \) and \( \mathbf{n}_\varepsilon \) at \( \varepsilon = 0 \).

For \( |\partial_\rho \mathbf{X}(\rho, \varepsilon)| \), we have

\[ \partial_\varepsilon |\partial_\rho \mathbf{X}(\rho, \varepsilon)| = \frac{\partial_\varepsilon \partial_\rho \mathbf{X}(\rho, \varepsilon) \cdot \partial_\rho \mathbf{X}(\rho, \varepsilon)}{|\partial_\rho \mathbf{X}(\rho, \varepsilon)|}, \]  

(A.3)

\[ \partial_\varepsilon^2 |\partial_\rho \mathbf{X}(\rho, \varepsilon)| = \partial_\varepsilon \left[ \frac{\partial_\varepsilon \partial_\rho \mathbf{X}(\rho, \varepsilon) \cdot \partial_\rho \mathbf{X}(\rho, \varepsilon)}{|\partial_\rho \mathbf{X}(\rho, \varepsilon)|} \right] \]

\[ \quad = \frac{\partial_\varepsilon \partial_\rho \mathbf{X}(\rho, \varepsilon) \cdot \partial_\rho \mathbf{X}(\rho, \varepsilon)}{|\partial_\rho \mathbf{X}(\rho, \varepsilon)|} - \frac{\partial_\varepsilon \partial_\rho \mathbf{X}(\rho, \varepsilon) \cdot \partial_\rho \mathbf{X}(\rho, \varepsilon) \partial_\varepsilon |\partial_\rho \mathbf{X}(\rho, \varepsilon)|^2}{|\partial_\rho \mathbf{X}(\rho, \varepsilon)|^3} \]

\[ = \frac{|\partial_\rho \mathbf{V}_0|^2}{|\partial_\rho \mathbf{X}(\rho, \varepsilon)|} - \frac{(\partial_\rho \mathbf{V}_0 \cdot \partial_\rho \mathbf{X}(\rho, \varepsilon))^2}{|\partial_\rho \mathbf{X}(\rho, \varepsilon)|^3}. \]  

(A.4)

Denote \( \mathbf{X} = \mathbf{X}(\rho, 0) \), take the value at \( \varepsilon = 0 \), and also note that \( \partial_\rho s(\rho, \varepsilon) = |\partial_\rho \mathbf{X}(\rho, \varepsilon)| \), we obtain

\[ \partial_\varepsilon |\partial_\rho \mathbf{X}(\rho, \varepsilon)| \bigg|_{\varepsilon=0} = |\partial_\rho \mathbf{X}| \partial_\rho \mathbf{V}_0 \cdot \mathbf{\tau}. \]  

(A.5)

\[ \partial_\varepsilon^2 |\partial_\rho \mathbf{X}(\rho, \varepsilon)| \bigg|_{\varepsilon=0} = |\partial_\rho \mathbf{X}| (|\partial_\rho \mathbf{V}_0|^2 - (\mathbf{\tau} \cdot \partial_\rho \mathbf{V}_0)^2). \]  

(A.6)
Thus we obtain the expansion of $|\partial_\rho X(\rho, \varepsilon)|$ at $\varepsilon = 0$

$$|\partial_\rho X(\rho, \varepsilon)| = |\partial_\rho X| \left[1 + (\tau \cdot \partial_s V_0)\varepsilon + \frac{1}{2} (\partial_s V_0 \cdot \partial_s V_0 - (\tau \cdot \partial_s V_0)^2) \varepsilon^2\right] + O(\varepsilon^3). \quad (A.7)$$

For $n^\perp = n(\rho, \varepsilon)$, note that we can express

$$n^\perp = -\frac{[\partial_\rho X(\rho, \varepsilon)]^\perp}{|\partial_\rho X(\rho, \varepsilon)|}. \quad (A.8)$$

So we have

$$\partial_\varepsilon n^\perp = -\frac{[\partial_\rho \partial_\rho X(\rho, \varepsilon)]^\perp}{|\partial_\rho X(\rho, \varepsilon)|} + \frac{[\partial_\rho X(\rho, \varepsilon)]^\perp \partial_\varepsilon |\partial_\rho X(\rho, \varepsilon)|}{|\partial_\rho X(\rho, \varepsilon)|^2}$$

$$= -\frac{[\partial_\rho \partial_\rho X(\rho, \varepsilon)]^\perp}{|\partial_\rho X(\rho, \varepsilon)|^3} + \frac{[\partial_\rho X(\rho, \varepsilon)]^\perp [\partial_\rho \partial_\rho X(\rho, \varepsilon) \cdot \partial_\rho X(\rho, \varepsilon)]}{|\partial_\rho X(\rho, \varepsilon)|^3}.$$

$$\partial_\varepsilon^2 n^\perp = \frac{[\partial_\rho \partial_\rho X(\rho, \varepsilon)]^\perp [\partial_\rho X(\rho, \varepsilon) \cdot \partial_\rho X(\rho, \varepsilon)]}{|\partial_\rho X(\rho, \varepsilon)|^3} + \frac{[\partial_\rho X(\rho, \varepsilon)]^\perp [\partial_\rho \partial_\rho X(\rho, \varepsilon) \cdot \partial_\rho X(\rho, \varepsilon)]}{|\partial_\rho X(\rho, \varepsilon)|^3}$$

$$+ \frac{3[\partial_\rho X(\rho, \varepsilon)]^\perp [\partial_\rho X(\rho, \varepsilon) \cdot \partial_\rho X(\rho, \varepsilon)]^2}{|\partial_\rho X(\rho, \varepsilon)|^3}. \quad (A.9)$$

Taking value at $\varepsilon = 0$, we obtain

$$\partial_\varepsilon n^\perp \bigg|_{\varepsilon=0} = -[\partial_\rho V_0]^\perp - n (\partial_s V_0 \cdot \tau). \quad (A.11)$$

$$\partial_\varepsilon^2 n^\perp \bigg|_{\varepsilon=0} = [\partial_\rho V_0]^\perp (\partial_s V_0 \cdot \tau) + (\partial_s V_0)^\perp (\partial_s V_0 \cdot \tau) - n (\partial_s V_0)^2 + 3n (\partial_s V_0 \cdot \tau). \quad (A.12)$$

Note that the expansion of $\gamma(n^\perp)$ at $\varepsilon = 0$ is given as

$$\gamma(n^\perp) = \gamma(n) + \nabla \hat{\gamma}(n) \partial_\varepsilon n^\perp \bigg|_{\varepsilon=0} \varepsilon$$

$$+ \frac{1}{2} (\nabla \hat{\gamma}(n) \partial_\varepsilon^2 n^\perp \bigg|_{\varepsilon=0} + H^\gamma(n) \partial_\varepsilon n^\perp \cdot \partial_\varepsilon n^\perp \bigg|_{\varepsilon=0}) \varepsilon^2 + O(\varepsilon^3). \quad (A.13)$$

Thus we immediately obtain the expansion of $\gamma(n^\perp)$ at $\varepsilon = 0$

$$\gamma(n^\perp) = \gamma(n) + \left[ -\gamma(n)(\tau \cdot \partial_s V_0) - \nabla \hat{\gamma}(n) \cdot (\partial_s V_0)^\perp \right] \varepsilon$$

$$+ \frac{1}{2} \left[ 2\nabla \hat{\gamma}(n) \cdot (\partial_s V_0 \cdot \tau)(\partial_s V_0)^\perp - \gamma(n)(\partial_s V_0 \cdot \partial_s V_0) \right.$$

$$+ 3\gamma(n)(\tau \cdot \partial_s V_0)^2 + H^\gamma(n)(\partial_s V_0)^\perp \cdot (\partial_s V_0)^\perp \left] \varepsilon^2 + O(\varepsilon^3). \quad (A.14)$$


[75] M.V. Laue, Der Wulffsche Satz für die gleichgewichtsform von kristallen, Z. Krystallogr, 105 (1943), 124-133


List of Publications


