

# RESEARCH STATEMENT

My research area is nonlinear partial differential equations with an emphasis on regularity issues and pattern formation.

## 1 Recent past work

### 1.0.1 Regularity problem from nonlinear elasticity

In [12, 76], We study the maximal smoothness for stationary states of the following variational integrals

$$(1.1) \quad I(u) = \int_{\Omega} \gamma(\nabla u(x)) dx.$$

Here  $\Omega \subset \mathbb{R}^2$  is a smooth bounded domain.  $u : \Omega \rightarrow \mathbb{R}^2$  and  $\gamma$  is a quasiconvex function satisfying  $\gamma = \infty$  when  $\det \nabla u < 0$ .

For domain variations of the form  $u_{\varepsilon}(x) = u(x + \varepsilon\varphi(x))$  for  $\varphi \in C_c^1(\Omega, \mathbb{R}^2)$ . The first variation in  $\varepsilon$  gives the *equilibrium equations*

$$(1.2) \quad \left( -\gamma \delta_{\alpha}^k + u_{x_k}^i \frac{\partial \gamma}{\partial P_{\alpha}^i}(\nabla u) \right)_{x_{\alpha}} = 0 \quad \text{in } \mathcal{D}'(\Omega)$$

for  $1 \leq k \leq 2$ .

In [76], we show that if  $u$  is a weak solution of (1.2) and if  $u \in W^{2,2} \cap C^1$ , then  $\det \nabla u$  is strictly positive in  $\Omega$  and  $u$  is smooth provided  $\gamma$  is smooth. We also present an example showing that the above result fails if we only assume  $u \in W^{2,r} \cap C^1$  for some  $r < 2$ .

In [12], we study an example used in [10, 76] and prove that this weak solution of (1.2) is a global minimizer in a large subset of all test functions. This is the first step in showing that certain special weak solutions to the equilibrium equations might be a global minimizer.

### 1.0.2 Sharp integral inequalities for harmonic functions

In [39], we consider the variational problem for  $1 < p < \infty$

$$(1.3) \quad c_{n,p}^{\frac{np}{n-1}} = \sup \left\{ \int_{\mathbb{R}_+^n} |Pf|^{\frac{np}{n-1}} dx : |f|_{L^p(\mathbb{R}^{n-1})} = 1 \right\}$$

with  $Pf(x) = \int_{\mathbb{R}^{n-1}} P(x, \xi) f(\xi) d\xi$  is the Poisson integral of  $f$ . We prove existence of maximizers and regularity properties of critical points. It was shown that all critical points are smooth, radially symmetric with respect to a point and strictly decreasing along radial direction. For special values  $p = \frac{2n}{n-1}$  and  $p = \frac{2(n-1)}{n-2}$ , exact forms of critical points are characterized.

In [40], we study the extension of the above problem to the case of compact manifold with boundary and prove similar properties for maximizers and critical points under suitable assumptions.

### 1.0.3 Existence and uniqueness of vortexless solutions for Chern-Simons-Higgs energy.

Let  $\Omega \subset \mathbb{R}^2$  be a bounded simply connected domain,  $\nabla_A = \nabla - iA$  where  $A \in \mathbb{R}^2$  and  $u : \Omega \rightarrow \mathbb{C}$ . In joint work with D. Spirn [63, 64], we consider the system of coupled elliptic PDE's:

$$(1.4) \quad -\frac{\mu_\varepsilon^2 |\operatorname{curl} A - h_{ex}|^2}{4|u|^4} u = \nabla_A^2 u + \frac{1}{\varepsilon^2} u (1 - |u|^2) (3|u|^2 - 1)$$

$$(1.5) \quad 0 = -\frac{\mu_\varepsilon^2}{4} \operatorname{curl} \left( \frac{\operatorname{curl} A - h_{ex}}{|u|^2} \right) + j_A(u).$$

Our main concern is existence and uniqueness of vortexless solutions to (1.4) – (1.5) in nonself-dual case  $\varepsilon \neq \mu_\varepsilon$ . In [63] we prove that for any given  $\varepsilon, \mu, h_{ex}$ , there exists a solution pair  $(u, A)$  of (1.4), (1.5). If  $\mu_\varepsilon \rightarrow 0$  satisfies  $\mu_\varepsilon \gg e^{-|\log \varepsilon|^\alpha}$  for any  $0 < \alpha < 1$ , there exists a critical field  $h_{c_1} = \frac{2|\log \varepsilon|}{\mu_\varepsilon^2}$  such that for  $h_{ex} \leq h_{c_1}$  the solution we obtained is vortexless. And for  $h_{ex} > h_{c_1}$ , our solution must have a vortex. Moreover, we [64] prove the existence of stable vortexless solutions to (1.4)-(1.5) for  $h_{ex} \leq C\varepsilon^{-\alpha}$  and  $\limsup_\varepsilon \mu_\varepsilon < \infty$ . Under the additional assumption that  $\mu_\varepsilon \geq \varepsilon^{\frac{1}{9}}$ , the stable vortexless solution obtained is unique among its class.

### 1.0.4 Higher order elliptic system

In [6, 7, 77], We study positive solutions for higher order elliptic system

$$(1.6) \quad \begin{cases} (-\Delta)^m u = |x|^a v^p \\ (-\Delta)^m v = |x|^b u^q \end{cases} \quad \text{in } \mathbb{R}^N.$$

For  $a = b = 0$ , we prove [77] there are no radial positive solutions if  $\frac{1}{p+1} + \frac{1}{q+1} > 1 - \frac{2m}{N}$  and for general case [7] there are no positive solutions to the system under the additional assumption that  $\max\left(\frac{2(p+1)}{pq-1}, \frac{2(q+1)}{pq-1}\right) \geq \frac{N-2m-1}{m}$ . In particular, if  $N = 2m + 1$  or  $2m + 2$ , there are no positive solutions if  $\frac{1}{p+1} + \frac{1}{q+1} > 1 - \frac{2m}{N}$ .

For  $a \geq 0, b \geq 0$ , we [6] prove there are no positive solutions with slow decay rates to higher order elliptic system (1.6) if  $p \geq 1, q \geq 1, (p, q) \neq (1, 1)$  satisfies  $\frac{1+\frac{a}{N}}{p+1} + \frac{1+\frac{b}{N}}{q+1} > 1 - \frac{2m}{N}$  and  $\max\left(\frac{2m(p+1)+a+bp}{pq-1}, \frac{2m(q+1)+aq+b}{pq-1}\right) > N - 2m - 1$ . Moreover, if  $N = 2m + 1$  or  $N = 2m + 2$ , this system admits no positive solutions with slow decay rates if  $p \geq 1, q \geq 1, (p, q) \neq (1, 1)$  satisfies  $\frac{1}{p+1} + \frac{1}{q+1} > 1 - \frac{2m}{N}$ .

### 1.0.5 Uniqueness of one dimensional Néel wall profiles

In joint work with Muratov [57], we prove uniqueness (up to translation) of monotone solutions of the following nonlocal equation

$$-\theta_{xx} + \cos \theta (\sin \theta - h) + \frac{\nu}{2} \cos \theta \left( -\frac{d^2}{dx^2} \right)^{1/2} \sin \theta = 0$$

subject to boundary constraints at infinity. Here  $\left(-\frac{d^2}{dx^2}\right)^{1/2}$  represents the linear operator whose Fourier symbol is  $|k|$ . This equation arises as the Euler Lagrange equation of the one dimensional reduced magnetic thin film energy. This result corresponds to uniqueness of one-dimensional Néel wall profiles. We also obtain some uniform estimates for general one-dimensional domain wall profiles.

### 1.0.6 Stability of a dislocation structure on low angle planar grain boundaries

Low angle grain boundaries can be modeled as arrays of line defects (dislocations) in crystalline materials. The classical continuum models for energetics and dynamics of curved grain boundaries are mainly based on those with equilibrium dislocation structures without the long-range elastic interaction, leading to a capillary force proportional to the local curvature of the grain boundary. The new continuum model recently derived by Zhu and Xiang [82] incorporates both the long-range dislocation interaction energy and the local dislocation line energy, and enables the study of low angle grain boundaries with non-equilibrium dislocation structures that involves the long-range elastic interaction. Using this new energy formulation, Xiang and PI ([75]) proved that the orthogonal network of two arrays of screw dislocations on a planar twist low angle grain boundary is always stable subject to both perturbations of the constituent dislocations within the grain boundary and the perturbations of the grain boundary itself.

### 1.0.7 Brezis-Nirenberg problem for fractional elliptic operators

In joint work with Chen and Montenegro [18], we study the existence and nonexistence of positive viscosity solutions of the following nonlocal Brezis-Nirenberg problem

$$(1.7) \quad \begin{cases} (-\mathcal{L})^s u = u^{\frac{n+2s}{n-2s}} + \lambda u & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

where  $(-\mathcal{L})^s$  denotes the fractional power of  $-\operatorname{div}(A(x)\nabla)$ ,  $0 < s < 1$ ,  $n > 2s$  and  $\lambda$  is real parameter. Assuming  $A(x) \geq A(x_0)$  for all  $x \in \bar{\Omega}$  and  $A(x) \leq A(x_0) + |x - x_0|^\sigma I_n$  near some point  $x_0 \in \bar{\Omega}$ , we prove existence theorems for any  $\lambda \in (0, \lambda_{1,s}(-\mathcal{L}))$ , where  $\lambda_{1,s}(-\mathcal{L})$  denotes the first Dirichlet eigenvalue of  $(-\mathcal{L})^s$ . Our existence result holds true for  $\sigma > 2s$  and  $n \geq 4s$  in the interior case ( $x_0 \in \Omega$ ) and for  $\sigma > \frac{2s(n-2s)}{n-4s}$  and  $n > 4s$  in the boundary case ( $x_0 \in \partial\Omega$ ). Nonexistence for star-shaped domains is obtained for any  $\lambda \leq 0$ .

### 1.0.8 Layer solutions for a one dimensional nonlocal model of Ginzburg-Landau type

In joint work with Chen and Muratov [19], we study a nonlocal model of Ginzburg-Landau type that gives rise to an equation involving a mixture of the Laplacian and half-Laplacian. Our focus is on one-dimensional transition layer profiles that connect the two distinct homogeneous phases. We first introduce a renormalized one-dimensional energy that is free from a logarithmic divergence due to the failure of the Gagliardo norm to be finite on smooth profiles that asymptote to different limits at infinity. We then prove existence, uniqueness, monotonicity and regularity of minimizers in a suitable class. Lastly, we consider the singular limit in which the coefficient in front of the Laplacian vanishes and prove convergence of the obtained minimizer to the solutions of the fractional Allen-Cahn equation.

## 1.1 A one dimensional nonlocal model of Ginzburg-Landau type with periodic translation invariance.

The proof of existence, monotonicity and uniqueness of minimizer in [19] relies on the fact that the renormalized one-dimensional energy is translation invariant. In joint work with Chen and Muratov [20], we consider minimization of the following nonlocal energy

$$(1.8) \quad \begin{aligned} J(u) &= \int_{\mathbb{R}} |u'|^2 + \int_{\mathbb{R}} (2 + \sin x) W(u) dx \\ &+ \int_{\mathbb{R}} \int_{\mathbb{R}} \left[ \frac{(u(x) - u(y))^2}{(x - y)^2} - \frac{(\eta(x) - \eta(y))^2}{(x - y)^2} \right] dx dy \end{aligned}$$

in the set

$$\mathcal{A} = \{u \in H_{\text{loc}}^1(\mathbb{R}) : u - \eta \in H^1(\mathbb{R})\}.$$

Here  $\eta(x) \in C^\infty(\mathbb{R})$  is a given function satisfying  $|\eta| \leq 1$ ,  $\eta(x) = 1$  for  $x \geq 1$ ,  $\eta = -1$  for  $x \leq -1$ .  $W(u)$  is a double well potential satisfies  $W(u) > 0$  if  $u \neq \pm 1$ ,  $W(\pm 1) = W'(\pm 1) = 0$  and  $W''(\pm 1) > 0$ . For the new model (1.8) with only periodic translation invariance, our previous argument fails and we need to seek new method. The main difficulty to prove existence of minimizer of (1.8) lies in two parts. Firstly, since  $\eta \notin H^{\frac{1}{2}}(\mathbb{R})$ , it is not a priori clear that  $J(u)$  is bounded from below on  $\mathcal{A}$ . Secondly, the energy bound does not necessarily imply the boundedness of  $u$  in a suitable sobolev space in general, therefore we can not apply direct method to yield a minimizer. To show  $J$  is bounded from below on  $\mathcal{A}$ , we divide the regions where  $u$  is close to  $\pm 1$  and where  $u$  is away from  $\pm 1$ . By carefully matching contributions from each region, all potential negative infinite energy is canceled out. To prove existence of minimizer, our main idea is as follows. Given an arbitrary minimizing sequence  $\{u_n\}$ , our will replace this sequence by another sequence  $\{\bar{u}_n\}$  constructed via reflecting negative parts of  $u_n$  outside suitable regions. Taking into account of our energy contribution estimates from lower bound argument, we can carefully choose the region where we do the reflection on  $u_n$  so that energy  $J(\bar{u}_n)$  differs slightly from  $J(u_n)$ . The sequence  $\{\bar{u}_n\}$  satisfies  $|u_n(x) + \text{sgn}(x)| \geq c > 0$  outside a uniformly bounded interval. For such a sequence, boundedness of energy implies boundedness of  $u_n - \eta$  in  $H^1(\mathbb{R})$ . From this and lower semicontinuity argument, we yield a limit function which attains minimum of  $J(u)$  in  $\mathcal{A}$ .

Our main result is the following existence and regularity theorem.

**Theorem 1** *There exists a minimizer  $u_0$  of  $J(u)$  in  $\mathcal{A}$ . Moreover,  $u_0 \in C^{2, \frac{1}{2}}(\mathbb{R})$  satisfies Euler-Lagrange equation*

$$-u_0'' - (2 + \sin x)W'(u_0) + 2\pi \left( -\frac{d^2}{dx^2} \right)^{\frac{1}{2}} u_0 = 0.$$

Here we understand the fractional operator in the following sense

$$\left( -\frac{d^2}{dx^2} \right)^{\frac{1}{2}} u_0(x) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\pi} \int_{|x-y| \geq \varepsilon} \frac{(u_0(x) - u_0(y))}{(x-y)^2} dy.$$

## 2 Future research

### 2.1 Low angle grain boundaries and dislocation climb model.

#### 2.1.1 Continuum models for low angle grain boundaries

A grain boundary is the interface where two single crystals of different orientation join in such a manner that the material is continuous across the boundary. Grain boundaries are a main feature of crystalline materials. They play an important role in determining the properties of materials such as creeping, weld cracking, electromigration resistance.

Dislocations are line defects in crystal structure. There are two main types of dislocations: edge and screw. An edge dislocation is a defect where an extra half plane of atoms is introduced (or removed) half way through the crystal. A screw dislocation corresponds to a rotation with respect to an axis which is perpendicular to the boundary plane. For edge dislocations, Burgers vector is parallel, while for screw dislocations, Burgers vector is perpendicular. A grain boundary consisting entirely of screw dislocations is called twist boundary and boundaries consisting entirely of edge dislocations are called tilt boundaries. Most of the grain boundaries in real materials consist of a network of both edge and screw dislocations.

We often separate grain boundaries by the extent of the misorientation between the two grains. Low angle grain boundaries (LAGBs) are those with a misorientation less than about 15 degrees. Such grain boundaries have relatively simple structure, their properties and structure are a function of the misorientation. In contrast the properties of high angle grain boundaries (HAGBs) whose misorientation is greater than about 15 degrees are normally found to be independent of the misorientation.

Under various forces acting on grain boundaries, the grain boundaries move and microstructure evolves. Grain boundary motion is the dominant factor for microstructural evolution process of polycrystalline materials such as grain growth, recrystallization. Due to the strong correlations among structure, energetics and dynamics of the grain boundaries, theoretical understanding of grain boundary migration is quite challenging. The classical model of low angle grain boundaries [41, 60, 65]. was derived for equilibrium planar grain boundaries consisting of regular arrays of straight dislocations and the dislocation structure is determined by Frank's formula [29, 41, 47, 60, 65]. The available continuum framework for dynamics of grain boundaries is based on the assumption that the capillary force is proportional to the curvature of the grain boundary. However, experiments and simulations [15, 16, 29, 42, 46, 47, 48, 49, 50, 51, 66, 68, 70] show that the migration on nonplanar low angle grain boundaries does not always follow Read-Shockley formula, its mobility strongly depends on the grain boundary structure.

Recently Zhu and Xiang [82] derived a continuum model for dislocation structure on low angle grain boundaries that are allowed to be nonplanar or nonequilibrium. Following the idea of a coarse-grained disregistry function (CGDF) introduced by Xiang [71, 81], they introduced a scalar dislocation density potential function on a grain boundary surface to describe the orientation dependent continuous distribution of dislocations with same Burgers vector. More precisely, consider a surface  $S$  consisting of dislocations with same Burgers vector  $\mathbf{b}$ , the dislocation density potential function  $\eta$  is a scalar function defined on  $S$  such that the constituent dislocations are given by its level set  $\eta = j$ . Under this definition, the local dislocation line direction is represented by

$$\mathbf{t} = \frac{\nabla_S \eta \times \mathbf{n}}{\|\nabla_S \eta\|}$$

and the inter-dislocation distance on  $S$

$$D = \frac{1}{\|\nabla_S \eta\|}.$$

Here  $\mathbf{n}$  is the unit normal vector of  $S$  and  $\nabla_S \mathbf{n} = \nabla \eta - (\mathbf{n} \cdot \nabla \eta) \mathbf{n}$  is the surface gradient of  $\eta$  on  $S$ . We consider  $J$  dislocation arrays on a low angle grain boundary  $S$  with Burgers vector  $\mathbf{b}^{(j)}$ ,  $j = 1, \dots, J$ . These arrays of dislocations are represented by dislocation density potential functions  $\eta_j$ ,  $j = 1, \dots, J$ . The continuum formulation of elastic energy of these dislocation arrays on  $S$  is given by

$$E_S(\eta, S) = E_{\text{long}} + E_{\text{local}},$$

where the long-range interaction energy

$$\begin{aligned} E_{\text{long}} = & \frac{1}{2} \sum_{i=1}^J \sum_{j=1}^J \int dS_x \int dS_y \left[ -\frac{\mu}{2\pi} \frac{(\nabla_{S_x} \eta_i(x) \times \mathbf{n}(x)) \times (\nabla_{S_y} \eta_j(y) \times \mathbf{n}(y)) \cdot (\mathbf{b}^{(i)} \times \mathbf{b}^{(j)})}{\|x - y\|} \right. \\ & + \frac{\mu}{4\pi} \frac{(\nabla_{S_x} \eta_i(x) \times \mathbf{n}(x) \cdot \mathbf{b}^{(i)}) (\nabla_{S_y} \eta_j(y) \times \mathbf{n}(y) \cdot \mathbf{b}^{(j)})}{\|x - y\|} \\ & \left. + \frac{\mu}{4\pi(1-\nu)} \left( \nabla_{S_x} \eta_i(x) \times \mathbf{n}(x) \times \mathbf{b}^{(i)} \right) \cdot \nabla_x \otimes \nabla_x \|x - y\| \cdot \left( \nabla_{S_y} \eta_j(y) \times \mathbf{n}(y) \times \mathbf{b}^{(j)} \right) \right]. \end{aligned}$$

and the local dislocation line energy

$$E_{\text{local}} = \sum_{i=1}^J \int_S \frac{\mu (b^{(i)})^2}{4\pi(1-\nu)} \left[ 1 - \nu \frac{(\nabla_{S_x} \eta_i(x) \times \mathbf{n}(x) \cdot \mathbf{b}^{(i)})^2}{(b^{(i)})^2 \|\nabla_S \eta_i(x)\|^2} \right] \|\nabla_S \eta_i(x)\| \log \frac{1}{r_g \|\nabla_S \eta_i(x)\|} dS_x.$$

Here  $b^{(i)} = \|\mathbf{b}^{(i)}\|$  and  $r_g$  is a parameter constant proportional to the dislocation core radius. The energy  $E_{\text{long}}$  represents the energy due to the long-range interaction of dislocations. The energy  $E_{\text{local}}$  is the local dislocation line energy. The dislocation line energy  $E_{\text{local}}$  dominates for equilibrium low angle grain boundaries (i.e. those satisfying Frank's formula); whereas both the long-range dislocation interactions and the local dislocation line energy play essential roles when the low angle grain boundaries are in nonequilibrium.

Under this formulation, considering the equilibrium state of the grain boundary  $S$  consisting of  $J$  dislocation arrays, the following equations hold:

$$(2.1) \quad \begin{aligned} \frac{\delta E}{\delta r} &= -\mathbf{f}_S^{\text{total}} \cdot \mathbf{n} = 0 \quad \text{when } \delta \mathbf{r} = \mathbf{n} \delta r \\ \frac{\delta E}{\delta \eta_j} &= \mathbf{f}_S^{(j)} \cdot \frac{\nabla_S \eta_j}{\|\nabla_S \eta_j\|} = 0, \quad j = 1, 2, \dots, J. \end{aligned}$$

The first one is the equilibrium with respect to the evolution of grain boundary  $S$ , the second one gives the equilibrium state with respect to the motion of the constituent dislocations on a fixed surface  $S$ . Here  $\mathbf{f}_S^{\text{total}}$  is the total force on the grain boundary  $S$  and  $\mathbf{f}_S^{(j)}$  is the force on the  $j$ -th dislocation array which can be written as  $\mathbf{f}_S^{(j)} = (\mathbf{f}^{(0)})^{(j)} + \mathbf{f}_{\text{lt}}^{(j)} + \mathbf{f}_{\text{p}}^{(j)}$ . The long-range Peach-Koehler force  $(\mathbf{f}^{(0)})^{(j)}$  comes from variation of the long-range energy  $E_{\text{long}}$  with respect to change of dislocation structure on  $S$ . The variation of the local dislocation line energy  $E_{\text{local}}$  with respect

to  $\eta$  gives two local forces  $\mathbf{f}_{\text{lt}}^{(j)}$  and  $\mathbf{f}_{\text{p}}^{(j)}$ . The force  $\mathbf{f}_{\text{lt}}^{(j)}$  is the local dislocation line tension force and  $\mathbf{f}_{\text{p}}^{(j)}$  is the local force in the direction normal to the local constituent dislocation.

Under this continuum framework, an orthogonal network of two equidistant straight arrays of screw dislocations on the twist boundary is represented by  $J = 2$ ,  $\eta_1(x, y) = \frac{y}{D}$ ,  $\eta_2(x, y) = -\frac{x}{D}$ . Here  $D = \frac{b}{\theta}$  is the interdislocation distance between two dislocation arrays sharing the same Burgers vector. Direct calculation show the long-range energy  $E_{\text{long}}$  vanishes and the local dislocation line energy  $E_{\text{local}} = \int_S \gamma dS$ , where

$$\gamma = \frac{\mu b}{2\pi} \theta \log \frac{b}{r_g \theta}.$$

This recovers the classical result on energy formula for a planar low angle twist boundary in discrete dislocation model [41, 60].

It is easy to check that the aforementioned  $\eta_i$  and  $S$  is an equilibrium point of (2.1). In a joint work with Xiang [75], PI used this continuum model and studied local stability of such orthogonal network of equidistant straight arrays on a planar grain boundary. Their work shows the second variation of the elastic energy with respect to the change of the grain boundary  $S$  and the change of dislocation structure on  $S$  are positive definite, which implies the local stability of such orthogonal network of dislocation array on planar grain boundaries.

For nonplanar static grain boundaries, finding the dislocation structure is not an easy task. Under this continuum framework, the motion of the grain boundary and evolution of the dislocation structure on the grain boundary is described by

$$(2.2) \quad \eta_{jt} = -m_j \frac{\delta E}{\delta \eta_j} = -m_j \left( \mathbf{f}_S^{(j)} \cdot \frac{\nabla_S \eta_j}{\|\nabla_S \eta_j\|} \right) \quad j = 1, 2, \dots, J,$$

$$(2.3) \quad v_n = -m_n \frac{\delta E}{\delta r} = m_n \sum_{j=1}^J \|\nabla_S \eta_j\| \mathbf{f}_S^{(j)} \cdot \mathbf{n},$$

where  $m_j > 0$  are mobility constants.

This continuum framework is general and applies to any dislocation arrays in three dimensions and includes both the long-range and short-range interaction between constituent dislocations. Based on this framework, Zhang, Gu and Xiang [79] established a continuum model to compute the energy of low angle grain boundaries for any given degree of freedom (arbitrary rotation axis, rotation angle and boundary plane orientation). Another application of this continuum framework is presented in [80]. They considered the problem where one cylindrical grain is embedded in another grain with arbitrary cross-section shape. The inner grain has a misorientation angle  $\theta$  relative to the outer grain and the rotation axis is parallel to the cylindrical axis. Assuming the cross-section curve of the grain boundary  $\Gamma$  is in the  $xy$ -plane and the rotation axis is in  $z$  direction. Expressing the closed curved grain boundary  $\Gamma$  in polar coordinates  $(R, \alpha)$ , the migration of  $\Gamma$  and evolution of dislocations on  $\Gamma$  can be written as a two dimensional problem

$$(2.4) \quad \frac{d\rho^{(j)}}{dt} = -M_d \left( \sum_{j=1}^J \frac{\rho^{(j)}}{\sqrt{R^2 + (R')^2}} \mathbf{f}_{\text{long}}^{(j)} \cdot \mathbf{T} \right)' - M_t \frac{\partial \gamma}{\partial \rho^{(j)}} - M_a \left( \frac{\rho^{(j)}}{|\rho^{(j)}|} \mathbf{f}_{\text{app}}^{(j)} \cdot \mathbf{T} \right)',$$

$$(2.5) \quad v_n = M_d \sum_{j=1}^J \frac{\rho^{(j)}}{\sum_{k=1}^J \rho^{(k)}} \mathbf{f}_{\text{total}}^{(j)} \cdot \mathbf{n} + M_b p.$$

Here  $\gamma$  is the grain boundary energy density,  $\mathbf{f}_{\text{long}}^{(j)}$ ,  $\mathbf{f}_{\text{app}}^{(j)}$  and  $\mathbf{f}_{\text{total}}^{(j)}$  are the forces on the dislocation with Burgers vector  $\mathbf{b}^{(j)}$  due to long-range interaction between dislocations, the applied stress field and the total force respectively.  $M_d$  is mobility of the dislocations and  $M_b$  is mobility associated with driving force due to the difference between the bulk energy densities of the two grains denoted by  $p$ .  $M_t$  and  $M_a$  are mobilities associated with the driving forces of the local energy and applied stress, respectively. Their model can be considered as a generalization of Cahn-Taylor model [15] by incorporating detailed formulas of the driving forces in the normal and tangential direction that depend on constituent dislocations, Burgers vectors and the grain boundary shape and shape change of the grain boundaries.

We propose to work on the following questions concerning the motion of grain boundaries and dislocations.

**A1.** Short time existence for initial value problem of equations (2.2) – (2.3) and (2.4) – (2.5).

One of the first question we ask is the well posedness. Given an initial grain boundary  $S(u, v, 0) = S_0(u, v)$ ,  $\eta_i(u, v, 0) = \eta_i(u, v)$ ,  $i = 1, \dots, J$ .  $\eta_i$  satisfies Frank's formula. Do we always have a unique solution  $S(u, v, t)$  and  $\eta_i(u, v, t)$  for (2.2) – (2.3) (respectively (2.4) – (2.5)) for  $t \in [0, T]$  for some  $T$ ?

The natural approach would be to formulate an implicit function theorem in a suitable space. Our initial step would be to calculate the linearization operator of the right hand side and check invertibility in a suitable function space. Due to the nonlocal feature of our energy, this is not so obvious. We expect to look into ideas of proof of local existence for harmonic heat flow problems. We remark that short time existence and uniqueness result as well as level set approach for a different dislocation dynamics have been addressed in [4]. Their model is a non-local eikonal equation on the characteristic function for the dislocation which is based on the model proposed by Rodney, Le Bouar and Finel [62].

**A2.** Level set formulation of equations (2.2) – (2.3) and (2.4) – (2.5).

To facilitate numerical simulations of dynamics of migration of grain boundaries, our next goal is to write the equation (2.2) – (2.3) (respectively (2.4) – (2.5)) into a level set formulation. The main idea of the level set method is to represent the moving interface  $\Gamma(t)$  (grain boundary  $S(t)$  in our case) as the zero level set of a Lipschitz continuous function  $\phi(\mathbf{x}, t)$ . The motion of  $\Gamma(t)$  can be written as an evolution equation for  $\phi$  as

$$\phi_t + V \|\nabla\phi\| = 0 \text{ given } \phi(\mathbf{x}, t) = 0$$

where  $\mathbf{V}$  represents the interface propagation speed. We expect to follow some ideas of level set formulation for some geometric evolution problems [28], which relies on coarea formula and proper identification on evolution speed of level surface.

**A3.** Self-similar solution to equation (2.2) – (2.3) and (2.4) – (2.5).

A further question to investigate next is to look into possible self-similar solutions to equation (2.2). By doing a dimensional analysis, we shall look for suitable scaling laws which will give us idea on how a self-similar solution look like. Our equations will be ode system in integral form, we might need to look into integral type odes for some ideas. New crystal image analysis recently developed in [78] may help us gain some better idea on identification of dislocations.

**A4.** Investigate other related models based on Zhu and Xiang’s framework.

Zhu and Xiang’s model has been generalized to three dimensions [83]. In this case, a pair of dislocation density potential functions (DDPFs) are introduced for each active slip system. The contour surfaces of DDPF  $\varphi$  describe the slip plane distribution and the other DDPF  $\psi$  identifies the density distribution of dislocation curves on the slip plane. In this formulation, the intersection of contour lines of integer multiples of the length of the Burgers vector of the two DDPFs are the locations of the dislocations. The plastic flow rule is described by evolution equations of DDPFs. Can we ask similar questions for this generalized model?

### 2.1.2 Dislocation climb model

Dislocation climb plays important roles in the plastic deformation of crystals at high temperatures [41]. Climb process is driven by the climb component of the Peach-koeher force on the dislocations and dislocations change slip planes by absorbing and/or emitting vacancies during the climb process. Many of the past works on dislocation climb dynamics [5, 8, 9, 22, 34, 38, 45, 55, 72, 73] were based on vacancy diffusion in the bulk and often Dirichlet boundary condition was adopted for the vacancy diffusion in the bulk. In those models, vacancy concentration along dislocation cores were assumed to be in equilibrium and climb velocity formulas were mainly expressed in terms of mobility law for a single, straight edge dislocation. (see [37] for climb velocity for curved dislocations and multiple dislocations in three dimensions) On the other hand, both pipe diffusion and absorption/emission of vacancies at the jogs on the dislocations play essential roles in the dislocation climb process.

Very few references in the literature have attempted to incorporate pipe diffusion and jog dynamics. For example, vacancy pipe diffusion was included in a three dimensional discrete dislocation dynamics model in [30] but vacancy diffusion in the bulk is neglected. Two limit cases associated with vacancy pipe diffusion were discussed in [22]. A multi-scale approach was proposed in [33].

Recently, Xiang et al [58] developed a mesoscopic dislocation dynamics model for vacancy assisted dislocation climb by upscalings from a stochastic model on the atomistic scale. Their model incorporated four microscopic mechanism involved in the dislocation climb process: i) bulk diffusion of vacancies, ii) vacancy exchange dynamics between bulk and dislocation core, iii) vacancy attachment-detachment kinetics at jogs and iv) vacancy pipe diffusion along the dislocation core. Under their formulation, the continuous spatial and time domains in consideration is  $\mathbb{R}^3 \times [0, \infty)$ , the dislocation is a jogged straight line nominally parallel to  $z$ -axis with core radius  $r_d$  and Burgers vector  $\mathbf{b}$  in the positive  $x$  axis. Let  $c^v(x, y, z, t)$  denote the vacancy concentration in the bulk at time  $t$ ,  $c^c(z, t)$  denote the vacancy concentration in the pipe. The vacancy bulk diffusion equation is

$$\begin{cases} c_t = D_v \Delta c \\ -\frac{\partial c}{\partial n} = \frac{1}{l_\phi} (c - c_d) \Big|_{r=r_d} \\ c = c_\infty \Big|_{r=r_\infty} \end{cases},$$

and climb velocity at any point on the dislocation is given by

$$\begin{aligned} v_{cl} &= \frac{2\pi r_d D_v}{bl_\phi} \left( \frac{1}{2\pi r_d} \int_{r=r_d} c \, dl - c_d \right) + D_c b \frac{d^2 c_d^c}{ds^2} \\ &= \frac{1}{b} \int_{r=r_d} \mathbf{j} \cdot \mathbf{n} \, dl + D_c b \frac{d^2 c_d^c}{ds^2}. \end{aligned}$$

Here  $l_\phi$  in the Robin boundary condition is a characteristic length that represents difference between the barrier for the vacancies hopping into the dislocation core from the bulk and that for the vacancy bulk diffusion.  $r_\infty$  is the outer cutoff for the distance to the dislocation.  $c_d$  and  $c_d^c$  are the average equilibrium vacancy concentrations on the dislocation core surface from outside and inside respectively and can be written as

$$c_d(z) = c_0 e^{-\frac{f_{cl}(z)\Omega}{bkT}}, \quad c_d^c(z) = c_0^c e^{-\frac{f_{cl}(z)\Omega}{bkT}},$$

with  $c_0 = e^{-\frac{E_v^f}{kT}}$  being the reference equilibrium vacancy concentration in the bulk and  $c_0^c = e^{-\frac{E_c^f}{kT}}$  being the reference equilibrium vacancy concentration in the dislocation core region. Here  $E_v^f$  and  $E_c^f$  are the vacancy formation energy in the bulk and within the dislocation core respectively.  $f_{cl}$  is the climb component of the Peach-Koehler force on the dislocation.  $k$  is Boltzmann's constant,  $T$  is the temperature,  $\Omega$  is the volume of an atom.  $s$  is the arc-length parameter along the dislocation. Under those notations, we have  $c_0 = k_v c_0^c$  where  $k_v$  is a dimensionless parameter indicating the difference between the hopping rates out of and into the dislocation core.

Using the new formulation, Xiang et al. [58] derived climb velocity formula for the special cases of a straight edge dislocation and a circular prismatic loop. In the limiting cases of negligible stress variation and fast exchange of vacancies between the dislocation and the bulk, their formula recovers classical climb velocity formula [41]. In particular, they considered prismatic loop at low temperature. It has been observed in experiments that the loop translate under a stress gradient and the vacancy bulk diffusion is negligible, i.e.  $D_v \approx 0$ . Under this condition, the climb velocity formula reduces to

$$v_{cl} = D_c b \frac{d^2 c_d^c}{ds^2}.$$

When  $f_{cl} \ll 1$ ,  $c_d^c \approx C f_{cl}$  for some constant  $C$ . Recall  $f_{cl} = -\kappa \log \sigma + O(1)$  with  $\kappa$  being the curvature of the object boundary and  $\sigma$  representing thickness of the region in which delta function of the object boundary is regularized [74], climb velocity formula in the sharp interface becomes

$$v_{cl} = C \frac{d^2 \kappa}{ds^2}.$$

This resembles the sharp interface formulation for Cahn-Hilliard equation with a concentration dependent mobility and this motivates us to ask the following question.

**A5.** Can we find a phase field formulation for this equation?

One of the main difficulty in finding a phase field formulation for this is due to the exponential expression of  $c_d^c$ . In joint discussion with Niu and Xiang, we obtained a phase field formulation through inner and outer expansions for the case where  $c_d^c = -c\kappa + g(s)$ . Is it possible to modify our argument to find a phase field formulation for  $c_d^c = \exp(-c\kappa + g(s))$ ?

## 2.2 Domain walls in ferromagnetic films.

Soft thin ferromagnetic films has been widely used as a data storage solution in modern technology. The related mathematical model has been extensively studied over the past 10 years. It is known that for sufficiently thin films, the magnetization vector almost lies entirely in the film plane. Film exhibits magnetic patterns consists of domains on which magnetization vector is almost constant.

Domains are connected by thin transition layers called domain walls along which magnetization vector changes rapidly from one direction to another.

The study of the domain wall structure has attracted a lot of attention. One of the common domain wall for thin film is Néel wall, in which the magnetization vector exhibit an in-plane  $180^\circ$  rotation between opposite magnetization. The structure of the Néel wall is rather well understood at current stage. Analysis based on micromagnetic arguments has been summarized nicely in books [1] and [43] (see also [54], [56], [61] etc). Experimental evidence of the one dimensional Néel wall profiles can be found in [11, 44, 69]. Rigorous mathematical analysis of Néel wall is more recent, starting from the work of García-Cervera [31, 32] on the analysis of the associated one dimensional variational problem. Melcher [52] studied the energy minimizer of the two dimensional reduced thin film model and obtained symmetry, monotonicity of the one dimensional minimizing profile as well as the logarithmic decay beyond the core region. Linearized stability of the one dimensional Néel wall with respect to one dimensional perturbations is proved in [17]. Asymptotic stability of one dimensional Néel wall with respect to large two dimensional perturbations is demonstrated in [27].

Recently, Chermisi and Muratov [21] studied the reduced one dimensional energy in the presence of an applied in-plane magnetic field applied in the direction normal to the easy axis. They expressed the magnetic energy in terms of the phase angle rather than the usual two-dimensional unit vector representation of the magnetization. They obtained uniqueness and strict monotonicity of the angle variable for the minimizing Néel wall structure. Moreover, they proved precise asymptotic behavior of the minimizing Néel wall profiles at infinity. The associated Euler-Lagrange equation in their setting is expressed as an ODE with a nonlocal term.

In joint work with C. Muratov [57], we follow the variational setting introduced in [21] and consider the critical point of the associated energy functional which is monotone. We prove that any monotone critical point of the reduced one dimensional energy is unique. Thus provide a better understanding of the numerical evidence presented in [56].

The energy functional related to such system, introduced by Landau and Lifschitz, can be written in CGS units as a combination of five terms, namely

$$(2.6) \quad \begin{aligned} E(\mathbf{M}) = & \frac{A}{2|M_s|^2} \int_{\Omega} |\nabla \mathbf{M}|^2 dx + \frac{K}{2|M_s|^2} \int_{\Omega} \Phi(\mathbf{M}) dx - \int_{\Omega} \mathbf{H}_{\text{ext}} \cdot \mathbf{M} dx \\ & + \frac{1}{2} \int_{\mathbb{R}^3} \int_{\Omega} \frac{\nabla \cdot \mathbf{M}(\mathbf{x}) \nabla \cdot \mathbf{M}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} dx dx' + \frac{M_s^2}{2K} \int_{\Omega} |\mathbf{H}_{\text{ext}}|^2 dx. \end{aligned}$$

Here  $\Omega \subset \mathbb{R}^3$  is the domain occupied by the ferromagnetic material,  $\mathbf{M} : \mathbb{R}^3 \rightarrow \mathbb{R}^3$  is the magnetization vector that satisfies  $|\mathbf{M}| = M_s$  in  $\Omega$  and  $\mathbf{M} = \mathbf{0}$  outside  $\Omega$ , positive constants  $M_s, A, K$  are the material parameters denoted as saturation magnetization, exchange constant and the anisotropy constant respectively,  $\mathbf{H}_{\text{ext}}$  is an applied external field, and  $\Phi : \mathbb{R}^3 \rightarrow \mathbb{R}$  is a nonnegative potential which vanishes at finitely many points.  $\nabla \cdot \mathbf{M}$  in the double integral is understood in distributional sense. The five terms in (2.6) represent the exchange energy, the anisotropy energy, the Zeeman energy, the stray-field energy and an inessential constant term added for convenience.

In the case of extended monocrystalline thin films with the in-plane easy axis we have  $\Omega = \mathbb{R}^2 \times (0, d)$ . Without loss of generality, we shall assume the easy axis is in the  $\mathbf{e}_2$  direction. Here  $\mathbf{e}_i$  is the unit vector in the  $i$ th coordinate direction. For moderately soft thin films, a *reduced thin film energy* has been derived [24, 25, 56], after significant reduction of energy. For a better

understanding of the parameter regime, we introduce the following quantities

$$l = \left( \frac{A}{4\pi M_s^2} \right)^{\frac{1}{2}}, \quad L = \left( \frac{A}{K} \right)^{\frac{1}{2}}, \quad Q = \left( \frac{l}{L} \right)^2$$

representing the exchange length, the Bloch wall thickness and the material quality factor respectively. For *ultra-thin* and *soft* film, we have  $d \lesssim l \lesssim L$  and at the same time balanced as  $Ld \sim l^2$ . We can then introduce a dimensionless parameter

$$\nu = \frac{4\pi M_s^2 d}{KL} = \frac{Ld}{l^2} = \frac{d}{l\sqrt{Q}}.$$

For reduced thin film energy, we can write

$$E(\mathbf{m}) = \frac{1}{2} \int_{\mathbb{R}^2} |\nabla \mathbf{m}|^2 + \frac{1}{2} \int_{\mathbb{R}^2} (\mathbf{m} \cdot \mathbf{e}_1 - h)^2 + \frac{\nu}{8} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \frac{\nabla \cdot \mathbf{m}(\mathbf{x}) \nabla \cdot \mathbf{m}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} dx dx',$$

where  $\mathbf{m} : \mathbb{R}^2 \rightarrow \mathbb{S}^1$  is the unit magnetization vector in the film plane.

We propose to work on the following problems.

**B1.** 2D stability of 1-D Néel walls.

Asymptotic stability of 1-D Neel wall with respect to 2-D perturbations which are periodic in  $x_2$  has been established in [27]. Their approach is based on a scaling law for the minimum energy. Dropping the anisotropy energy, they consider the thin film approximation of (2.6) in the following form

$$(2.7) \quad E_{x_1 x_2 \text{thin}}(m') = d^2 t \int_{\mathbb{R} \times (0, w)} |\nabla' m'|^2 + \frac{t^2}{2} \int_{\mathbb{R} \times (0, w)} \left| |\nabla'|^{-1/2} \nabla' \cdot m' \right|^2 dx'.$$

Where  $x' = (x_1, x_2)$ ,  $m'(x_1, x_2) = (0, \pm 1)$  for  $\pm x_1 \geq w_{\text{tail}}$  and  $m'(x_1, x_2 + w) = m'(x_1, x_2)$ ,  $w_{\text{tail}}$  being the tail width for Néel wall. It is shown that the energy of ultra-thin Néel wall behaves like

$$E_{\text{Neelthin}} \approx \frac{\pi}{2} t^2 \ln^{-1} \frac{t w_{\text{tail}}}{d^2} \approx \min \frac{1}{w} E_{x_1 x_2 \text{thin}}(m'),$$

in the regime  $d^2 t^{-1} \ll w_{\text{tail}}$ , thus the 1d Néel wall is asymptotically optimal.

We shall attack the 2-D stability of 1-D Neel wall differently. We first look at local stability with respect to 2-D perturbations. In joint work with Christof Melcher and Cyrill Muratov [53], we achieved the following local stability result on 1-d Néel wall.

**Lemma 2** (*local stability*) *If  $\theta = \theta(x_1)$  is a one dimensional Néel wall subject to center and boundary conditions  $\theta(0) = 0$  and  $\theta(\pm\infty) = \pm \frac{\pi}{2}$ , then  $\text{Hess}(E_0(\theta))(\varphi, \varphi) \geq 0$  for any  $\varphi$  compactly supported in  $\mathbb{R}^2$  and  $\varphi(0, 0) = 0$ .*

To study stability of 1-D Néel wall under large 2 dimensional perturbations, we look at the following model problem

$$(2.8) \quad -\Delta u + (-\Delta)^{\frac{1}{2}} u - \sin u (\cos u - h) = 0 \text{ in } \mathbb{R}^2,$$

where  $u : \mathbb{R}^2 \rightarrow \mathbb{R}$  is a bounded function satisfying  $\frac{\partial u}{\partial x_1} > 0$  in  $\mathbb{R}^2$  and  $\lim_{x \rightarrow \pm\infty} u(x_1, x_2) = \pm 1$ . We proved  $u$  is a function of one variable using some ideas from work on layer solutions of sum of fractional Laplacians such as paper by Cabre and Serra [14].

Can we apply this to study the stability of 1-D Neel wall under large two dimensional perturbations? The main challenge is how to handle the nonlocal term in the original setting.

**B2.** Get a better understanding of 2d domain wall structures such as cross-tie walls.

While 1-d Néel wall structure is relatively well understood, 2d domain wall structures are less studied. One typical 2d wall structures observed in ferromagnetic thin films is cross-tie walls. Cross tie wall is a periodic pattern of small-angle Néel walls with period  $w_{cross}$  which macroscopically acts as  $90^\circ$  walls. Experiments indicate the cross-tie wall move closer together with increasing anisotropy. It is also observed in experiments that  $w_{cross}$  decreases as film thickness  $t$  increases. However, a rigorous theory on mechanisms predicting the value of  $w_{cross}$  is still lacking. Based on the observation that the cross tie wall resembles an ensemble of Néel walls, a heuristic argument on internal length scale for cross tie wall is developed in [26]. Their main conclusion is that the internal length scale of cross tie wall should be determined by the repulsive interaction of Néel wall tails. How can we make this rigorous?

Another interesting problem is the transition between different domain walls as thickness of film varies. Cross tie wall is often observed in intermediate regime ( $t \sim d$ ), the transition from Néel wall to cross tie wall then to asymmetric Bloch wall as thickness of film increases has been observed both experimentally [36, 43] and in numerical simulations [67]. In the regime  $Q \ll t^2 d^{-2} \ll Q^{-1}$ , under the assumption that the magnetization is independent of the tangential in-plane variable  $x_2$  (i.e.  $m = m(x_1, x_3)$ ), transition from a Néel wall to an Asymmetric Bloch wall as thickness increases has been classified in [59]. Using a scaling law argument, they rigorously identified the transition by establishing the cross-over in the specific wall energy. Can we get a similar scaling law analysis for this transition for the full three dimensional model? The scaling law argument relies on the matching upper bounds and lower bounds. While the upper bounds are relatively easy using the known ansatz, the matching lower bound which is ansatz free is always more difficult. A related work on cross tie wall is [3] where they identified the exact form of a cross tie pattern as a minimum state for a sharp interface model. How do we adjust their argument to get a similar lower bound by matching the parameters? Can we combine the heuristic idea in [26] and the rigorous argument in [3] in a suitable way to get a rigorous explanation on  $w_{cross}$ ?

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