The Hong Kong University of Science and Technology

Department of Mathematics


# PhD THESIS EXAMINATION

# Stochastic and Deterministic Peierls-Nabarro Models with Gamma-surface in Complex Crystal Systems

*By*


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***ABSTRACT***

This thesis comprehensively studies both deterministic and stochastic Peierls-Nabarro models for dislocations in complex crystal systems. Dislocations are line defects in crystalline materials, and understanding their behavior is crucial for understanding plastic deformation properties in these materials. Peierls-Nabarro models are a type of continuum model used to simulate dislocations, which incorporate atomistic structures within the dislocation core region. This approach enables simulations at larger length and time scales. Specifically, we examine two complex cases for the Peierls-Nabarro model: complex lattices, which are unions of simple lattices like graphene, and high-entropy alloys, which are single-phase crystals with random solid solutions of five or more elements of nearly equal composition. High-entropy alloys are widely believed to possess many ideal engineering properties.

In the first part, we prove the convergence of the atomistic model to the deterministic Peierls--Nabarro model for a complex bilayer system with second-order accuracy. Using low-degree polynomials, we approximate the energy based on atomistic interactions of different groups of atoms and demonstrate the consistency and stability of the Peierls--Nabarro and atomistic models.

In the second part, we derive stochastic continuum models for high-entropy alloys with short-range order from atomistic models. The proper continuum limit obtained preserves the mean and variance of the atomic level randomness and the short-range order characterized by a characteristic length. The resulting continuum model with short-range order is validated using an Ornstein-Uhlenbeck (OU) process, previously adopted phenomenologically for high-entropy alloys with short-range order. Stochastic continuum models with short-range order are derived for elasticity in high-entropy alloys without defects and high-entropy alloys with dislocations (line defects), based on energy formulations, whose variations lead to stochastic partial differential equations.

In the third part, we present stochastic elastic models for high-entropy alloys, derived from atomistic models in a two-dimensional system. Using asymptotic analysis and limit theorem, we obtain a stochastic Hooke's law that approximates the elastic strain energy in a plane-strain problem. The formula for stochastic Hooke's law in high-entropy alloys takes the form of anisotropic elasticity, while it is expressed in isotropic form in terms of expectation. Our method includes the random terms in point defect theory of high-entropy alloys.

The obtained results offer theoretical support and mathematical insight for Peierls-Nabarro models, aiding in the understanding of the behavior of high-entropy alloys at both the atomic and continuum levels.


**Date : 7 July 2023, Friday**

**Time : 3:00 pm**

**Venue : Room 4472 (Lifts 25/26)**

***Thesis Examination Committee*:**

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***(Open to all faculty and students)***

**The student's thesis is now being displayed on the reception counter in the General Administration Office (Room 3461).**