

Analysis and Numerics of Variational Models for Kinematically Incompatible Elasticity

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論 文 名	Analysis and Numerics of Variational Models for Kinematically Incompatible Elasticity (運動学的に不適合な弾性に関する変分モデルの解析と数値解析)		
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論 文 審 査 の 結 果 の 要 旨

The thesis is divided into two parts. The first focuses on applying the calculus of variations to solid mechanics problems, particularly the investigation of frustration and stress fields arising from lattice mismatches. The second part presents research from an internship at Daicel Corporation, where computational chemistry was used to optimize chemical properties in molecular machines. A foundational theme of the thesis is the role of compatibility conditions in elasticity. These conditions, first formulated in the 19th century by Saint-Venant, Beltrami, Michell, and others, ensure that mechanical strains arise from a single-valued displacement field. However, topological defects such as dislocations and disclinations can violate these conditions. This was first rigorously studied by Volterra, who identified dislocations as translational defects and disclinations as rotational asymmetries. The mathematical treatment of such defects has since led to significant advancements in calculus of variations, including connections to the Ginzburg–Landau theory, harmonic maps, liquid crystals, and the topological degree theory for Sobolev maps. Building on this foundation, recent work by Cesana, De Luca, and Morandotti (SIMA, 56(1), 2024) has developed a general variational framework to model systems of disclinations (both isolated and in dipoles). However, modeling systems that simultaneously include disclinations and dislocations remains an open problem.

In Chapter 2 of the thesis—based on a joint paper with P. Cesana and M. Morandotti currently under review—the candidate proposes the first variational framework capable of simultaneously modeling regularized systems of wedge disclinations and edge dislocations. This work is set in the context of planar elasticity with linearized kinematics. The main contribution lies in providing a rigorous variational characterization of mechanical equilibrium in systems with incompatible strains. For non-simply connected domains, it is shown that the equilibrium problem for non-liftable strain–stress fields can be reformulated as a well-posed minimization problem involving the Airy stress potential. This scalar reformulation presents a significant advantage, enabling the analysis of dislocation–disclination systems through a well-posed variational principle. The approach opens the door to studying asymptotic behaviors (e.g., homogenization, relaxation, and coarse-graining) through the scalar Airy framework, bypassing the more complex original tensorial equations. Moreover, it is shown that this minimization problem can be reduced to a finite-dimensional optimization involving cell formulas. This has important implications for simplifying numerical computations and understanding

homogenization in dislocated crystalline structures.

In subsequent chapters, the candidate addresses modeling and analytical challenges in Föppl–von Kármán (FvK) plates exhibiting both translational and rotational incompatibilities. The FvK equations describe moderately large deflections in thin plates and are widely used in structural mechanics. Applications include the modeling of metal plates and graphene sheets affected by the presence of dislocations and disclinations. Prior literature has often introduced additional phenomenological phase-field variables to model plasticity without a clear derivation of the driving forces or underlying mechanisms. In Chapter 3, the candidate derives FvK equations incorporating a finite number of wedge disclinations, collaborating with Cesana and Baldelli. While similar models exist, questions of existence and regularity remained open; these are addressed through new existence theorems, adapting Ciarlet’s results in compatible elasticity. The chapter also includes a numerical implementation in FEniCS using a Discontinuous Galerkin method with C0 elements, suitable for 4th-order problems, with energy-based penalization to tune parameters. An application demonstrates a snap-through transition involving four disclinations, showing that the critical transition distance is approximately independent of the elastic parameters. Chapter 4 presents novel contributions on the mathematical analysis of regularized FvK plates with both disclinations and dislocations. The core-radius regularization method—originally developed for dislocations by Cermelli and Leoni (SIAM, 2005) and extended to disclination dipoles by Cesana, De Luca, and Morandotti (SIMA, 2024)—is further extended here to nonlinear FvK plates. The main difficulty lies in the nonlinearity introduced by the Monge–Ampère operator coupling the Airy potential with plate deflection and the non-convex, min–max variational structure of the problem. The candidate establishes an existence theorem for equilibrium configurations, characterizing them as saddle points of a non-convex energy functional in both the Airy potential and deflection. The analysis follows the lines of the proof of von Neumann’s min–max theorem, combined with compactness techniques adapted from Ciarlet’s work. The analysis is presently restricted to fixed core-radius $\varepsilon > 0$, leaving open the question of deriving a limiting model as $\varepsilon \rightarrow 0$.

The final chapter presents the candidate’s internship at Daicel Corporation, focusing on computational chemistry for bandgap optimization in diarylethene molecular switches. These molecules are promising for nanoscale electronic switching and have applications in materials science and photonics. The work aligns with the broader goals of the U.S. "Materials Genome Initiative" launched in 2011. The candidate developed a computational platform combining Density Functional Theory software with an in-house genetic algorithm. This system iteratively optimized molecular structures through random substitutions and selection, leading to the discovery of new diarylethene derivatives with enhanced bandgap properties. The candidate’s contributions are substantial, well-documented, and diverse—spanning mathematical theory, numerical implementation, and industrial application. The research has already led to the publication of two peer-reviewed papers—one in the *International Journal of Quantum Chemistry*, and one in *Applied Mathematical Modelling*—with a third under review at the *Journal of Elasticity*. Taking into account all the above, we acknowledge that the candidate deserves to be awarded the degree of Doctor of Functional Mathematics.