Modeling of Solid-to-Solid Phase-Transformations in Shape-Memory Alloys Homogenization and Gamma-Convergence Problems for Nematic Elastomers

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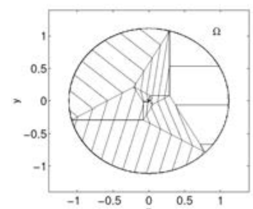
As a mathematician and an engineer, my research interests span the application of mathematical modeling and analysis techniques to a variety of materials science problems inspired by experimental observations and technology. More specifically, I have a keen interest in microscale phenomena such as pattern formation and topological singularities occurring in soft matter and elastic crystals. Knowledge of the microscopical features of a multifunctional material and understanding their interactions on the overall macroscopic properties is of strategic importance in the design of materials for engineering applications. Two specific lines from my past and current research are summarized below.

1) Modeling of solid-to-solid phase-transformations in shape-memory alloys

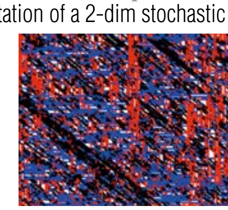
Martensitic phase transformation is observed in various metals, ceramics and biological systems. Shape-memory alloys are most important for technological application. Although there is vast potential to the shape-memory effect, practical implementations have been slow, and to-date, limited to Ni-Ti due to various reasons. It is strategically important to improve and stabilize the shape-memory effect in known materials and develop new modeling strategies. A problem I have been studying is the analysis and modeling of disclinations, a type of topological defects of the crystalline structure. Disclinations as those of Fig. 1-a are characterized by a self-similar tripole-star pattern resulting in localized concentration of mechanical stress. Mathematically, it can be shown that such configurations arise as a solution of differential inclusion problems related to 2-dimensional 3-spin systems. By identifying the basic algebraic structure underlying the models of n-state spin systems it has been possible to shed light on the mechanism that drives formation of a closed loop created by matching different crystal variants including a singularity. This project liaises with strategic national research endeavours in Japan in the area of multifunctional materials synthesis and design. Furthermore, I have been collaborating with probabilists on the modeling of the space-time evolution of the microscopic structure of an elastic crystal as a stochastic process. Here the modeling strategy consists in describing the growth and evolution of martensitic variants as a branching random walk process (see Fig. 1-b). The question that I want to address is the behavior of certain features of the self-similar structure thus formed and the computation of distribution laws for the interfaces of a given length. A portion of this research plan requires collaboration with experimentalists from the labs of Prof. Planes and Prof. Vives from the University of Barcelona on the validation of the above mentioned models with experimental observations. The ultimate goal of this multidisciplinary research effort is the understanding of the key activation mechanisms that drive avalanches in metals thus shedding some light on the dynamics of solid-to-solid phase-transformations.

Fig. 1

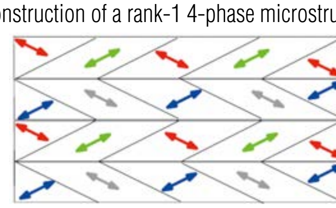
a) Self-similar tripole-star patterns observed in $Pb_3(VO_4)_2$ and MgCd resulting from the rotation of twin boundaries and linking of different crystal variants.



b) Numerical computation of a 2-dim stochastic microstructure.



c) analytical construction of a rank-1 4-phase microstructure in NLCEs.



2) Homogenization and Gamma-Convergence problems for nematic elastomers

Amongst biocomposites with the most promising perspective, Nematic Liquid Crystal Elastomers (NLCEs) combine the entropic elasticity of a network of cross-linked polymeric chains with the peculiar optical properties of nematic liquid crystals. A thorough understanding of the manipulation of optical birefringence in thin-films of NLCEs by mechanical, electric and thermal means is a tremendous task and could create new opportunities across a broad spectrum of fundamental sciences. Focusing on the strain-order coupling, my research sheds some light on the current understanding of mechanisms that rule the low energy states of mechanically constrained NLCEs, as in artificial muscles and lenses. The mathematical language required to tackle these problems is calculus of variations and especially Gamma-convergence. This sophisticated technique is at the intersection of analysis of PDEs and functional analysis based on an energy approach which is particularly suitable for the study of singularly perturbed problems. In the future, I wish to develop a research platform to achieve a comprehensive analysis of the intricate phenomena regarding coupling of order, elasticity and electric fields involving collaborations at experimental level as well.