様　式　Ｃ－１９、Ｆ－１９－１、Ｚ－１９　（共通）

科研費 KAKENHI

科学研究費助成事業　　研究成果報告書

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研究課題名（和文）Bridging across mathematical analysis, probability and materials mechanics for a better modeling of martensitic microstructure and defects.

研究課題名（英文）Bridging across mathematical analysis, probability and materials mechanics for a better modeling of martensitic microstructure and defects.

研究代表者
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交付決定額（研究期間全体）：（直接経費）　　3,300,000円

研究成果の概要（和文）：The purpose of the research plan is the development of mathematical theories to investigate the emergence of instabilities and defects at very small scales in classes of materials relevant for technological applications, such as, Shape-Memory Alloys and soft crystalline biopolymers.

研究成果の学術的意義や社会的意義
The modeling work has bridged across analysis (disclinations described as solutions to differential inclusions) and probability (description of self-similarity via branching random walks). This mathematical work has complemented the experimental work performed in Japanese laboratories.

研究成果の概要（英文）：The purpose of the research plan is the development of mathematical theories to investigate the emergence of instabilities and defects at very small scales in classes of materials relevant for technological applications, such as, Shape-Memory Alloys and soft crystalline biopolymers. Regarding soft polymers, I have accomplished the full analysis of Nematic Elastomers in the elastic-foundation geometry (a configuration relevant for sensors and actuators) clarifying all the possible energy and order states. In metallurgy-related problems, on one hand, I have introduced continuum and atomistic models for describing formation of topological defects in the lattice of elastic crystals based on the variational principle and computed exact solutions for non-linear models under special symmetry assumptions. On the other hand, I have introduced probabilistic models to study martensitic transformations as a fragmentation process and found power law behavior which is in agreement with experiments.

研究分野：Calculus of Variations

キーワード：Non-linear analysis　Materials Science　Gamma-convergence　Stochastic processes

１．研究開始当初の背景

Nematic Elastomers. The research on the modeling of elastic foundations with rigorous tools of calculus of variations has been pioneered in AAL Baldelli, B. Bourdin, *J. Elas.* 121, 2015 where the first rigorous derivation of Winkler foundations has been obtained with rigorous asymptotic analysis of energy principles (Gamma-convergence, homogenization of elliptic vectorial PDEs and relaxation). However, this analysis is limited to homogenous materials with no active microstructure. In the direction of functional materials, the classical result on active thin films is the paper by Y.C. Shu, *ARMA,* 153, 2000 where the effective (mesoscale) energies of thin Shape-Memory (martensitic) films is computed at all relevant length-scales. However, Shu's analysis is limited to homogenized structures (that is, under the restriction that the admissible microstructure has to be periodic and material relaxation is ruled out) and no elastic foundation-type of coupling is considered.

Disclinations. Despite the mechanics of disclinations (rotational lattice defects) has been extensively studied with the classical methods and concepts of non-linear hyper-elasticity since the '70s (de Wit, Fressengeas, Romanov), a rigorous and comprehensive theory based on variational principles has been elapsing. This is a major dichotomy, for instance, with the case of dislocations (translational lattice defects) which have been object of intensive mathematical analysis based on the variational principle. There appears to still be a gap in the mathematical modeling of disclinations especially on the development of variational methods based on energy minimization.

Mathematical modeling of **martensite** has been essentially confined, since the pioneering work of J. Ball, R. James, *ARMA* 100, 1987, to the development of a variational theory based on the application of concepts of homogenization and relaxation to the crystallographic theory of martensite. A monumental body of work emerged since the '80s has clarified the mechanism driving formation of martensitic microstructure by means of energy minimization and kinematic compatibility. However, this approach leaves many un-answered questions, such as, the mechanisms driving formation of martensitic microstructure and emergence of self-similarity. Indeed, experimental evidence has shown occurrence of power-law behavior and universality during the nucleation of martensite from austenite (A. Planes, L. Manosa, E. Vives, *J.A. Compounds* 577-1, 2013). A first physics paper (Torrens et al., *PRE*, 95, 2017) has proposed a modeling approach inspired by Bak's ideas on self-organized criticality based on a simple probabilistic fragmentation model. However, a mathematical modeling approach based on rigorous limiting arguments and derivation of general shape theorems for random variable has been missing.

Symmetry methods have been classically applied to 2^{nd}-order non-linear PDEs yielding exact solutions even when no variational structure is present. Typical cases are represented by Allen-Cahn, Ginzburg-Landau or Fitzhugh-Nagumo type equations which find application as phase-field models for various chemical processes and 2-phase physical systems. However, very few exact solutions are available for time-dependent multi-dimensional 4^{th}-order non-linear reaction diffusion equations.

２．研究の目的

The purpose of the research project has been the development of a platform of mathematical models and techniques to study solid-to-solid (and, more in general, multi-) phase transformations in various classes of smart materials, including soft elastic crystals (nematic elastomers) and shape-memory alloys (martensite). My research plan has complemented the work of domestic groups and laboratories on the experimental investigation of smart materials. In particular, collaborations have been established and are still on-going with the lab of Prof. K. Urayama (Kyoto Tech) on the modeling of nematic elastomers experiments under torsion and of Prof. T. Inamura (Tokyo Tech) on the analysis of power-law behavior in martensite and on the modeling of disclinations with variational methods. From the point of view of the materials, I have investigated various type of mechanical instabilities and defects observed at small scales, that is, nano- (disclinations in homogenous lattices as well as in martensite) and micro-meters (shear bands and wrinkles in nematic elastomers) as well as avalanches and self-similar features occurring over a span of several decades. From the theoretical point of view, my research plan has bridged over mathematical analysis, elasticity theory and probability in a unified effort to better understand the behavior of materials for technological applications.

３．研究の方法
The research plan has entailed theoretical investigation borrowing tools and theories from various branches of mathematics and theoretical physics.

Probabilistic methods based on the Crump-Mode-Jagers theory for **Branching Random Walks** have been adopted for the modelling of the space-time evolution of a fragmentation scheme mimicking a martensitic microstructure. Exact asymptotic properties for the limiting random variables have been obtained and compared with the statistics from numerical realizations of the fragmentation model encoded in Matlab.

Self-similar microstructures constructed over a lattice in an elastic crystal have been modelled by using the language of **differential inclusions** and by generalizing techniques developed in: S. Conti, M. Klar, and B. Zwicknagl, *Proc. R. Soc. A*, 473 (2017).

Wedge planar disclinations have been modelled as rotational mismatches over a triangular lattice and have been analysed with the tools of **Calculus of Variations**. I have performed exact analysis of the asymptotics of an atomistic model and computed its continuum limit by means of Gamma-convergence. Numerical codes have been prepared and the energy of the lattice models have been obtained and compared with results already known from the literature. Nematic elastomer in the geometrical regime of thin elastic foundations has been modelled with the language of linearized elasticity.

Analytical tools exploiting special **symmetry** structure of non-linear 4^{th} order PDEs have been developed to construct exact solutions for general models of phase-transformations.

４．研究成果
(1) **Nematic Elastomers (NEs)**
Accomplished exact analysis of sandwich structures of NEs with applications in the modeling of experimental configurations of active elastic foundations.

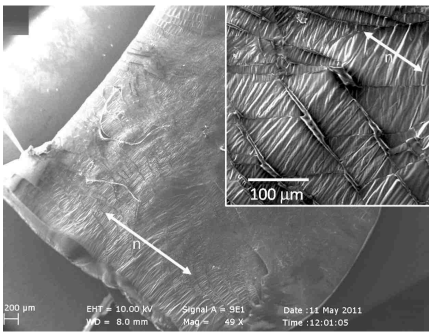


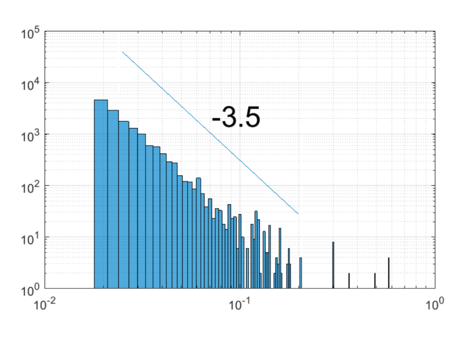
Image taken from: P. Cesana, AAL Baldelli, Variational modelling of nematic elastomer foundations, *Mathematical Models and Methods in Applied Sciences*, 2863-2904, Vol.28, 2018

Computed the exact effective energy of a system composed of a homogeneous elastic film deposited on a thin NE foundation and anchored to a rigid substrate. Possible applications of this analysis are in the design of electro-mechanical sensors based on the interplay of dielectric microstructure, elasticity and geometry. I discovered that a mesoscale model of NE foundation is represented by a 2D integral functional interpreted as a linear membrane on top of a nematic active foundation involving an effective De Gennes optic tensor allowing for low order states. The latter can suppress shear energy by formation of microstructure as well as act as a pre-strain transmitted by the foundation to the overlying film. An application of this modeling result is numerical analysis based on the Finite Element Method of NEs in various geometries and mechanical regimes, including planar membranes and plates.

(2) **General mathematical theories of phase-field models for phase-transformations.**
Constructed exact multi-dimensional time-dependent solutions for a 4^{th}-order Allen–Cahn–Hilliard equation by using the nonclassical symmetry of nonlinear reaction–diffusion equations. Obtained similarity solutions of a 4^{th}-order nonlinear partial differential equation for axisymmetric surface diffusion by extending an inverse method previously used for the second-order one-dimensional nonlinear diffusion equation. Developed an optimization algorithm to construct a well- defined mobility function that is effectively a single-valued function of surface orientation. One paper published and another submitted for publication (currently under review):

P. Broadbridge, D. Triadis, D. Gallage, P. Cesana, Nonclassical symmetry solutions for 4^{th}-order phase field reaction diffusion, *Symmetry*, 10, p.1-18, 2018
P. Broadbridge, D. Triadis, D. Gallage, P. Cesana, Solution for the 4^{th}-order non-linear axisymmetric surface diffusion by inverse method *(under review)*.

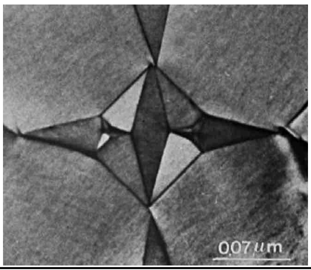
(3) **Self-similar microstructures in martensite**



Computed exact power law exponents for the asymptotic distribution of length of interfaces. Developed a platform of numerical codes for the simulation of fragmentation experiments and the statistical processing of the data generated. Results are in qualitative agreement with experimental data available in the literature. On-going work on the quantitative comparison with experimental data of power law exponents obtained from T. Inamura's Lab (Tokyo).

One paper submitted for publication (currently under review):
P. Cesana, B.M. Hambly, A probabilistic model for interfaces in a martensitic phase transformation, https://arxiv.org/pdf/1810.04380.pdf

(4) **Martensitic microstructure and disclinations**



Developed a mathematical theory for the description of self-similar microstructures as the solution to differential inclusion problem. Discussed an application of this theory to the kinematic description of martensitic disclinations as well as for the construction of exact solutions in the theory of NEs. This constitutes the starting point for an energy-minimization approach and a stability analysis of lattice disclinations.

Image taken from: C. Manolikas, S. Amelinckx, Phase transitions in ferroelastic lead orthovanadate as observed by means of electron microscopy and electron diffraction, *Phys. Stat. Sol.* (a) 60, p.607–617, 1980.
One book chapter (with no credits to the grant) published and one preprint:
P. Cesana, Relaxation of an energy model for the triangle-to-centred rectangle transformation, chapter in the book: The role and importance in innovation. Proc. of the Forum "Math for Industry", Springer, Mathematics for Industry Book Series p.117-126 (10 pages), Vol. 25, 2016.
P. Cesana, F.D. Porta, A. Rueland, C. Zillinger, B. Zwicknagl, Exact constructions in the (non-linear) planar theory of elasticity https://arxiv.org/abs/1904.08820

(5) Accomplished the variational modeling of **wedge disclinations** as the continuum limit of atomistic models. Constructed a platform of numerical codes for the computation of equilibrium configurations and energies. Comparisons with results available from the literature are in good agreement. One paper in preparation in collaboration with P. van Meurs (Kanazawa).

Collaborations established during the tenure of the grant have led to the submission of **successful research grant applications**, among which

1. AiRIMaQ fellowhip granted by Kyushu University (~Y2.3M)
2. RIMS Grant to host a Gasshuku-style conference (~Y1.2M)
3. Kakenhi Innovative Area (~Y3.6M)

５．主な発表論文等　　　　　Main presentation papers etc.
〔雑誌論文〕（計２件）　2 **peer-reviewed** papers (+3 preprints)

1. P. Cesana, AAL Baldelli, Variational modelling of nematic elastomer foundations, *Mathematical Models and Methods in Applied Sciences*, p.2863-2904, Vol.28, 2018
2. P. Broadbridge, D. Triadis, D. Gallage, P. Cesana, Nonclassical symmetry solutions for 4^{th}-order phase field reaction diffusion, *Symmetry*, 10, p.1-18, 2018

〔学会発表〕（計 21 件）21 invited seminars/conferences
"Models for disclinations in martensite": 1) U. Cambridge (March 2019); 2) OIST Okinawa

(January 2018); 3) Conference on dislocations and interfaces; 4) Fukuoka (August 2017); 5) U. Barcelona (June, 2017); 6) U. Swinburne (March 2017); 7) CNRS-IMSIA Lab Paris (December 2016); 8) Conference on Hysteresis, Avalanches and Interfaces, Oxford (September 2016); 9) Workshop of self-interacting processes, U. Monash (September 2016)

"Models and analysis of nematic elastomer membranes" 10) AIMS conference Taipei (July 2019); 11) Impact Workshop, Fukuoka (February 2018); 12) Workshop on Free Boundaries, Melbourne (September 2018); 13) U. Muester (June 2017); 14) U. Kanazawa (April 2017); 15) U. Monash (March 2017); 16) NIMS Tsukuba (February 2017); 17) RMIT (January 2017); 18) U. Queensland (November 2016); 19) U. Melbourne (October 2016); 20) MSI Colloquium, Australian National University (October 2016); 21) U. La Trobe (May 2016).

〔図書〕（計１件）　　1 book chapter (grant is uncredited)
P. Cesana, Relaxation of an energy model for the triangle-to-centred rectangle transformation, chapter in the book: The role and importance in innovation. Proc. of the Forum "Math for Industry", Springer, Mathematics for Industry Book Series p.117-126 (10 pages), Vol. 25, 2016.

〔産業財産権〕
○出願状況（計０件）

名称：　　　N.A.
発明者：　　N.A.
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種類：　　　N.A.
番号：　　　N.A.
出願年：　　N.A.
国内外の別：N.A.

○取得状況（計０件）

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〔その他〕
ホームページ等.　　https://pierluigicesana.weebly.com/research.html
https://www.imi.kyushu-u.ac.jp/eng/academic_staffs/view/163

６．研究組織

(1)研究分担者
研究分担者氏名：

ローマ字氏名：

所属研究機関名：

部局名：

職名：
研究者番号（８桁）：

(2)研究協力者
研究協力者氏名：
ローマ字氏名：

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