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Report on doctoral thesis by Mr. Gabriel Pathó
"Mathematical modeling of thin films of martensitic materials"

1 General information

Mr Gabriel Pathó has completed his PHD thesis under the supervision of Doc. RNDr. Martin Kružík. The thesis are concerned with problems around mathematical and computer modeling of thin films of martenstic materials. The main contribution are four papers:

[1] (with B. Benešová and M. Kružík) A mesoscopic thermomechanically coupled model for thin-film shape-memory alloys by dimension reduction and scale transition;

[2] Modelling of Thin Films of Shape-Memory Alloys;

[3] (with B. Benešová and M. Kružík) Young measures supported on invertible matrices;

[4] (with J. Krämer, S. Krömer and M. Kružík) $\mathcal{A}$-quasiconvexity at the boundary and weak lower semicontinuity of integral functionals.

They are dealing with the modeling and the rigorous mathematical description of shape memory effects in the material science by undertaking the two approaches:
(A) *Papers [1] and [2]:* Mathematical modeling, analysis and numerical verifications of thin films in martensitic materials, including theoretical methods to deal with the related complicated systems of pde's;
(B) *Papers [3] and [4]:* Theoretical approach to investigate lower semicontinuity properties of energy functionals which appear in many branches in the material science, among them those which describe shape memory behavior. The papers are using modern tools from calculus of variations, among them gradient Young measures and convex integration.

To my opinion the problem of investigation of shape memory alloys is one of the central problems in the material science, being at the same time extremely interesting within the group of several specialists: mathematicians, physicists, engineers and chemists. From mathematical point of view it is interesting at the same time in the applied branch, as well as in the theoretical one, because of the challenging problems appearing there. In the theoretical part the problems are on the borderline of pde's, calculus of variations and functional analysis. To contribute there one has to be well acquainted not only with the theoretical classical background, but also has to follow recent related literature in many areas, among them: modeling (because of successive improvements and verifications of the models), pde's (because of the new tools appearing like for example new variants of measure valued solutions) and calculus of variations (for example the usage of rather recent results from convex integration theory).

The articles have been published in the well recognized journals (Continuum Mechanics and Thermodynamics, Applicable Analysis, Advances in the Calculus of Variations). One of them, paper [2] - written by the author alone, is published in Technische Mechanik because of its special character - the implementation of the specific model. In many cases the methods are based on techniques from papers of Tomas Roubicek, Martin Kruzik and coauthors. Every article addresses interesting open problems and proposes perspectives for further investigations in both: the applied and the theoretical branch.

The final effect of dissertation: derivation and further analysis of the model with the emphasis on thin film techniques and contribution to the existence theory for energy minimizers has been achieved with the success.

2 Overview of the thesis

The dissertation consists of five chapters, first of them has the introductory character, while Chapters 2-5 contain papers [1]-[4], respectively.

Introduction is well written, interesting and provides the comprehensive information from physics, modeling and mathematics. It helps the nonspecialist to understand the background, motivations, as well as the important mathematical tools used in the preceding sections and can serve as the independent source of the supporting knowledge.

Chapter 2 contains paper [1]. It deals with the macroscopic thin-film model for the shape memory materials. The novelty of the approach is taking into account the thermomechanical effects based on the model proposed by T. Roubiček and B. Benešová in 2012. The authors apply it to the spatial geometry of thin films, by using the dimension reduction techniques. As the result they obtain existence of weak solutions to the macroscopic model. What can me mentioned: the authors use the variational approach, the functionals are defined on the anisotropic Sobolev and BV-type spaces. One has to use the solid analysis, because of complicated systems of pde's appearing. Moreover, the passage to the macroscopic model requires the implementation of Young measures and leads to weak solutions which involve Young measures in its definition. Contribution in this paper requires the good knowledge from pde's, calculus of variations, recent literature, and very good technical skills.

Chapter 3 contains paper [2], which was written by Mr. Patió alone. He analyzes the static martensitic thin-film model in the shape-memory-alloy proposed by Bhacharaya and James in 1999. The model has been applied to the Ni-Mn-Ga single crystal and the demonstration was inspired by the previous work of M. Kružík and T. Roubiček from 2004. The issue involves the nonconvex variational functionals defined on gradients of Sobolev functions. For their analysis the author uses laminates known in the theory of micristructures, applies gradient Young mesures introduced by D. Kinderlehrer and P. Pedregal to control the Γ limits of the related energy functionals. The analysis of Γ limits is related to the technique of dimension reduction. The theoretical tools have been implemented to the numerical verification. As mentioned by the author at the end of the work, it is possible to extend this work in many other directions, for example to the dissipative evolutionary models.

Chapter 4 presents paper [3]. It deals with the tools needed to the study of minimization problems where the energy functionals involve integrands defined on invertible matrices. One of the tools is the quasiconvexity property of the integrands which in that case have to be discontinuous along rank-one matrices. The standard relaxation techniques have to be adjusted to the usage of specific Young measures. Those are the measures which are generated by sequences of gradients

of Sobolev mappings such that that both: the gradients and gradients of their inverse functions are controlled in L^p. As an effect of this werk one obtains the characterization of such Young measures. The interesting nonstandard ingredient is the implementation of one theorem known in convex integration theory, when dealing with the case $p = \infty$. The contribution in this paper requires good knowledge in functional analysis and many technical skills. The work is very well motivated by elasticity theory and is the valuable contribution to the theory of Sobolev mappings with invertible gradients. It is also the pioneering contribution to the theory of gradient Young measures which are controlled by discontinuous functions.

Last part, *Chapter 5* deals with functionals defined on gradients of $\mathcal{A}$-free vectorfields where $\mathcal{A}$ is the given first order vector-valued differential operator of constant rank, where no boundary type condition on minimizing sequence is given. It is based on methods developed by I. Fonseca, M. Kružík, S. Krömer, and coauthors. The issue requires the new notion, which is $\mathcal{A}$-quasiconvexity at the boundary, being the generalization of the classical convexity at the boundary introduced by J.M. Ball and J. Mardsen in 1984. As one of main effects the authors obtain characterization of integrands which are $\mathcal{A}$-quasiconvex at the boundary and apply them to study lower semi-continuity of the related functionals. Interesting open questions are addressed at the end of the paper. They are related to the extension properties of function spaces of $\mathcal{A}$-free vectors defined on domains. The contribution in this work requires a lot of knowledge from the general theory of Sobolev spaces (one uses for example the theorem about projection of periodic vectorfields onto the $\mathcal{A}$-free ones) and technical skills.

To my opinion the thesis are nontrivial, interesting and require a lot of knowledge from applied analysis, pde's, mathematical modeling, numerics, the classical theory of Sobolev spaces, calculus of variations, functional analysis, recent related literature, a lot of technical skills. The contribution in such research field makes the mathematician the really good expert.

From critical remarks: it would be better if the author had more papers written alone. This situation is however justified by the very ambitious problem undertaken, which required a lot of cooperation.

3 Final conclusion

Taking into account the provided discussion I confirm that the presented thesis meets all customary and statutory requirements imposed for doctoral dissertations and prove Mr. Gabriel Pathó's ability to the creative scientific work in the future.

Sincerely yours,

Agnieszka Kałamajska