Dear Professor Dr. Zdeněk Němeček,

Univerzita Karlova V Praze,
Matematicko-Fyzikální Fakulta,
Ke Karlovu 3,
12116 Praha 2,
Česká Republika

Pavia, August 16, 2012

Ref: Referee report on the PhD thesis by Barbora Benešová

Dear Professor Němeček,

Let me start by expressing my gratitude to you and the Subject Board of the Faculty of Mathematics and Physics for the consideration. I am pleased of having received the possibility of reviewing the PhD thesis by Barbora Benešová which I regard to be very interesting and well-written.

The thesis focuses on a new model for shape-memory alloys. The latter are metallic alloys which exhibit two amazing thermo-mechanical behaviors known as the superelastic and the shape-memory effects. These two macroscopic effects are the result of a thermal and stress-driven structural phase change in the crystalline phase of the materials. The result of this phase change is often the formation of very specific micro-structural patterns of the various crystal variants of the material. Up to now, the description of such a microstructure in the evolutive case has been elusive to a sound mathematical treatment. The model considered in this thesis is specifically tailored in order to contribute in this very relevant direction. Benešová's thesis focuses on advancing a new mesoscopic model for the quasi-static thermo-mechanic evolution of shape-memory single crystals along with a specific description of the corresponding microstructure. Existence analysis for suitably weak solutions and the development of a series of numerical experiments are also reported. Although some materials have been already presented in publications by Barbora Benešová, also in collaboration with Martin Kružík, Tomaš Roubíček and Gabriel Pathó, the thesis contains also original results.

The thesis is organized in seven chapters. A quite accurate although essential introduction to shape-memory alloys phenomenology is given in Chapter 1 together with some reference to standing modeling ideas. Chapter 2 contains instead a collection of mathematical tools which are later needed in the proofs.
In particular, Chapter 2 stands as an introduction to the general theme of relaxation of non-convex functionals in Mechanics, with a specific emphasis on Young measures, also by referring to some new and personal results in the field. Chapter 3 instead is focusing on the general frame of thermomechanical modeling for so-called generalized standard materials, namely the reference setting for the proposed model. A brief account of the current available mesoscopic models for shape-memory alloys is then given in Chapter 4. The core of the thesis is contained in Chapter 5 where the new model is advanced, some suitable notion of weak solvability is introduced and the corresponding existence is proved twice. In particular, the mentioned weak solution is firstly obtained as a suitable limit of microscopic solutions by taking into account interfacial energies between the crystal variants. Physically this corresponds to a large-body limit. Secondly, the same existence result is obtained via a suitable time-discretization scheme. The latter serves as the basis for the numerical treatment. Chapter 6 records some more specific analytical results which can be obtained by requiring the mechanical energy of the medium to be convex. Although quite restrictive, this setting is still of some interest as the corresponding analysis is more flexible. Finally, Chapter 7 reports on a number of numerical tests aimed at assessing the amenability of the model in some reference boundary-value configurations.

I regard the results of the thesis as very interesting and new. The description of microstructure thermo-mechanical evolution in shape-memory alloys is clearly an extremely challenging task. Although necessarily biased by a number of modeling simplifications, Benešová’s thesis is bringing an undisputed novel approach to it. To my view, the crucial idea of the modeling consists in introducing a double descriptor of the microstructure in terms of a Young measure and of the local phase fractions (scalar). The ideal linear constraint between these two can be then relaxed, at the benefit of actually coupling the evolution of deformation and enthalpy solely through the mentioned phase fraction variable. This is particularly advantageous from the analytical side as it results in a better-tamed coupling of the energy conservation equation with the mechanical evolution.

The analytical part of the thesis is rooted upon some fairly technical a-priori-estimation strategies, also relying on the celebrated technique by Boccardo and Gallouët for parabolic equations with integrable source terms. The occurrence of the rate-dependent evolution of the enthalpy calls for some modification of previous existence theories. In particular, I found very interesting the selection of a cluster point argument in § 5.4.3 and the alternate minimization procedure from § 5.5.1. My impression is that both these ideas could be profitably exported to different situations. Moreover, let me explicitly mention the side-results of § 2.3.2 on Young measures generated by invertible matrices. I regard this perspective to be very promising in connection with the standing difficulty of framing the relevant convexity and growth notions for elasticity. The numerical tests presented are quite interesting and, I believe, demonstrating the ability of the model to produce reasonable predictions. The main idea here is the use of a backtracking strategy in order to regulate conservation of energy at the discrete level. This has the net effect of reducing the complexity of the incremental minimization problem: one sorts out a sequence of local incremental minima by means of a global energy-quasi-conservation argument.
I regard this to be a nice tool, although I cannot exactly see if it would be possible to develop some convergence analysis for it.

Finally, it is worth mentioning that the thesis is well-written and a quite enjoyable read. In particular, I appreciated the effort in presenting the general discussion of the first chapters as well as the care in explicating the arguments in the key analytical chapters.

In conclusion, I rate the work done by Benešová to be of very high quality. This thesis definitely proves Benešová's abilities in the direction of creative scientific work and I have hence no hesitations in strongly supporting her promotion.

Kind regards,

Ulisse Stefanelli

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