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Referee Report on the Doctoral Thesis of Vojtěch Kulvait
"Mathematical analysis and computer simulations of deformation of nonlinear elastic bodies in the small strain range", Mathematical Institute of Charles University

The doctoral thesis is devoted to power-law models of nonlinear theory of elasticity exhibiting an implicit constitutive response in the regime of small strain. The principal feature is that volumetric and deviatoric parts of the response tensor are separated. The investigation deals with modelling and mathematical analysis of the nonlinear elasticity problems supported by fitting experimental data for titanium alloys and by reporting numerous data of numerical simulation in the anti-plane setting of the problem.

The thesis is good written. It is 171 pages in length and consists of two introductory Sections 1 and 2; the main body: Section 3 on the modelling of alloys, Section 4 on the mathematical analysis, Section 5 on the numerical simulation; and Appendix containing basic definitions.

In the introduction, there is presented an overview of the literature and the history of mathematical modelling in solid mechanics of nonlinear constitutive responses of power and exponential type. The general formulation (1) of a static elasticity problem is introduced with the stress-strain response constituted in implicit form $\boldsymbol{\varepsilon} = \mathbf{G}(\mathbf{T})$, where $\boldsymbol{\varepsilon}$ is the linearized strain and $\mathbf{T}$ is the Cauchy stress tensors. The author splits it in the trace and the deviatoric part which are of power type such that

$$\mathrm{tr}(\boldsymbol{\varepsilon}) = \frac{1}{3K}\left(\frac{\tau_K^2 + |\mathrm{tr}(\mathbf{T})|^2}{\tau_K^2}\right)^{\frac{s'-2}{2}} \mathrm{tr}(\mathbf{T}), \quad \boldsymbol{\varepsilon}^{\mathrm{d}} = \frac{1}{2\mu}\left(\frac{\tau_\mu^2 + \|\mathbf{T}^{\mathrm{d}}\|^2}{\tau_\mu^2}\right)^{\frac{q'-2}{2}} \mathbf{T}^{\mathrm{d}} \qquad (2.20)$$

with material parameters K, μ, τ_K, τ_μ and finite exponents $s', q' > 1$. The limit case $s' = q' = 1$ implies a limiting small strain model extensively studied by J. Málek and K.R. Rajagopal with co-authors. It is worth to note that the other case of exponents $s' = q' = 2$ turns the constitutive model into the standard linearized elasticity law.

In Section 3, the implicitly constituted power laws (2.20) are fitting newly developed beta phase titanium alloys like gum metal. The experimental data up to strains of 2.5% under uniaxial tensile stress are extracted by Plot Digitizer from those figures available in the engineering literature. The bulk K, shear μ, and Young's E elastic moduli of the studied titanium alloys are estimated using Voigt, Reuss, and Voigt-Reuss-Hill approximations. To estimate the model parameters τ_K, $\tau_\mu = \sqrt{\frac{2}{3}}\tau_K$, s', q', the following nonlinear (NL) approaches are utilized. The best fit by maximizing the coefficient of determination R^2 measured in a linear regression analysis under either NLB - Bulk response condition (3.27) or the reverse NLS - Share response condition which leads to auxetics with negative Poisson's ratio ν, and NLO - by maximizing an Objective function (3.30) which improves R^2 with Voigt and Reuss estimates of ν. The fit results are extensively documented in numerous tables and figures.

In Section 4, a weak variational formulation of the nonlinear elasticity problem (1) is obtained in Lebesgue and Sobolev function spaces for a continuous, monotone, and coercive constitutive function **G**. The author applies an elliptic regularization in the form (4.21) and establishes its solvability using Galerkin's approximation on finite-dimensional subspaces. Based on a-priori estimates, passing to the limit in the regularization parameter, there exists an accumulation point implying a solution of the reference variational problem for the particular power-law response **G** from (2.20). A generalized Korn's inequality suitable for deviatoric strains was used here.

In the largest Section 5, numerous results of computer simulation implemented in Python on the FEniCS open-software platform are reported in the anti-plane setting of the problem under traction loading. The corresponding Airy stress function satisfies a nonlinear Dirichlet problem (5.14). The problem is examined over two-dimensional non-smooth domains excluding either V-shaped notch of the opening angles $\alpha \in \{1°, 2°, \dots, 180°\}$ with the sharp tip, or V-O-shaped notch with a circle at the tip, or V-C-shaped notch with a smoothened tip. For illustration of singular solutions, there are presented the exponents of singularity of the strain k_ε and of the stress $k_\mathbf{T}$ at the sharp V-notch tip, which are known from the literature for a simplified power-law model.
In the notched computational domain, the author applies conforming finite elements based on piecewise-continuous second-order polynomials on generated in COMSOL adaptively refined grids in the range of $3{\cdot}10^3$ - $5{\cdot}10^5$ DOF. For simulation, three types of titanium alloys are estimated by the NLB, NLS, and NLO models from Section 3. The large amount of numerical experiments was carried out and performed selectively in tables and figures in dependence on the model parameters. Because the power exponent q' and μ by data fitting are different between various models, there are certain differences in the numerical performance, especially for the NLO model describing auxetics.

I have no any negative remarks, rather few comments for possible future work:

1. The Dirichlet problem (5.14) is of the minimal hypersurface type due to I. Ekeland, R. Temam, *Convex Analysis and Variational Problems*, SIAM, 1999 (Chapter V, Section 3, Problem (3.4)-(3.5)).
2. For the singularity exponents k_ε, $k_\mathbf{T}$ in the limiting small strain model, see M. Zappalorto, F. Berto, K.R. Rajagopal, On the anti-plane state of stress near pointed or sharply radiused notches in strain limiting elastic materials: closed form solution and implications for fracture assessements. *Int. J. Fract.* (2016), 199, p.169-184.
3. Due to my personal interest to crack problems, it would be of interest the numerical simulation of the anti-plane problem for a crack when the notch angle $\alpha = 0°$.
4. Computer simulation of the power-law constitutive equation in the plane setting of the problem sure would be of great interest in the community.

The doctoral thesis submitted by Mgr. Vojtěch Kulvait provides a major contribution to the field of applied mathematics and physics. It fulfils the requirements for a dissertation in the highest degree. I sure recommend the acceptance and grade the work with "very good" (outstanding performance).

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