CMM-SolMech 2022 conference

S05 Micromechanics of heterogeneous materials

List of abstracts

ID 27: *Granular computing in computational homogenisation problems* (poster) – W. Beluch, M. Hatłas, J. Ptaszny

ID 38: *Space-fractional Kirchhoff-Love plate theory for bending analysis with scale effect* – P. Stempin, W. Sumelka

ID 42: *Experimental analysis and numerical modelling in the framework of fractional calculus of self-healing phenomena in roofing felts* – B. Łuczak, W. Sumelka

ID 49: *Microstructure and modeling of austenitic stainless steels during fracture at cryogenic temperatures* – E. Schmidt, B. Skoczeń, K. Nalepka

ID 59: *Impact of fibre orientation distribution reconstruction accuracy on composite's behaviour prediction* – W. Ogierman

ID 60: *Effect of twinning on void growth and the lattice orientation heterogeneity in HCP single crystals* – S. Virupakshi, K. Frydrych, K. Kowalczyk-Gajewska

ID 63: *Application of mechanical equivalence hypothesis to composite effective properties estimation* – A. Wiśniewska, H. Egner

ID 65: *Stress-strain behaviour of metal cellular materials using artificial neural networks* – A. Stręk, M. Dudzik, T. Machniewicz

ID 75: *Modelling of plastic deformation of metal crystals by a quasi-extremal energy principle* – M. Kursa, H. Petryk

ID 86: *Experimental and multiscale characterization of elastic viscoplastic copper under cyclic loading* – G. Girard, K. Frydrych, K. Kowalczyk-Gajewska, M. Martiny, S. Mercier

ID 89: *The effect of inclusion spatial distribution: modelling and experimental validation* – K. Kowalczyk-Gajewska, K. Bieniek, M. Maj, M. Majewski, K. Opiela, T. Zieliński

ID 93: *Moving layers and graded damage coupling with elasto-plasticity* – C. Stolz

ID 102: *Fractional calculus in material instability for non-local solids* – P. Beda

ID 117: *Contact analysis of branched crack surfaces by the Boundary Element Method* – P. Fedeliński

ID 129: *Towards optimal space-fractional Euler-Bernoulli beam design* (poster) – K. Szajek, P. Stempin, W. Sumelka

ID 141: *Shear band formation in porous thin-walled tubes subjected to dynamic torsion* – A. Vishnu, J. C. Nieto-Fuentes, J. A. Rodriguez-Martinez

ID 146: *Mesoscopic simulations of fracture in RC beams using DEM* – M. Nitka, J. Tejchman

ID 167: *Microstructural modeling of anisotropic and tension-compression asymmetric ductile metals* – S. Hashem, N. Hosseini, G. Vadillo

ID 172: *Analysis of composites with interphases* – H. Altenbach, L. Nazarenko, H. Stolarski

MODELLING OF PLASTIC DEFORMATION OF METAL CRYSTALS BY A QUASI-EXTREMAL ENERGY PRINCIPLE

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Solving of rate-independent polycrystal or single crystal plasticity problems is related to non-uniqueness of incremental solutions. The main difficulty in the crystal plasticity problems arises from indefinite and non-symmetric slip-system interaction matrix when a set of active slip-systems at a material point level has to be determined. The solution and the set of active slip-systems can be found using the computational approach based on the incremental energy minimization [1]. In order to find the solution using the incremental energy minimization, the selective symmetrization of the slip-system interaction matrix restricted to active systems has been proposed. However, a generic rate-problem in crystal plasticity is of non-potential type. The question arises how to select a physically meaningful solution among multiple possibilities when the known extremal principles do not apply.

The new concept to predicting the time-independent response of metal crystals is based on the recently proposed quasi-extremal energy principle (QEP) [2]. The quasi-extremal energy principle enables finding the solution to a generally non-potential problem. The main advantage with the respect to the previous computational approach to rate-independent crystal plasticity problems [1] is that the present approach does not require any symmetrization of the slip-system interaction matrix.

The computational algorithm originally developed for step-by-step minimization of the incremental energy supply, under the symmetry restriction imposed on the constitutive law, is now modified in order to solve the QEP problem. The minimization method applied to solve the QEP problem is based on the augmented Lagrangian method and is implemented within the Wolfram Mathematica environment.

The effectiveness of the modified algorithm is demonstrated by examples of the large deformation of a fcc single crystal under simple shear and uniaxial tension. The approach enables step-by-step selection of the current set of active slip-systems. It is shown that a numerically stable solution can be found for which the number of simultaneously active slip systems does not exceed five. The QEP results are compared to those obtained using approach based on the selective symmetrization and also those of conventional rate-dependent framework. Especially with the simulations in a high-symmetry initial orientation, where several equivalent solutions exist, significant differences are visible. Moreover, the numerical simulations have been compared to the available experimental results, showing the benefits of using the computational approach based on QEP.

[1] Petryk H., Kursa, M. Incremental work minimization algorithm for rate-independent plasticity of single crystals. Int. J. Num. Meth. Engng. 104: 157-184, 2015.
[2] Petryk H. A quasi-extremal energy principle for non-potential problems in rate-independent plasticity. J. Mech. Phys. Solids 136: 103691, 2020.