Structure-Based Optimization of Crystal Plasticity Parameters in Metals and Alloys

K. Frydrych^{1,2} and S. Papanikolaou¹

 ¹ NOMATEN Centre of Excellence, National Centre for Nuclear Research, Świerk-Otwock, Poland
² Institute of Fundamental Technological Research, Polish Academy of Sciences, Warsaw, Poland E-mails: kryd@ippt.pan.pl

The crystal plasticity (CP) theory enables to include the microstructural information about the plastic deformation mechanisms (such as dislocation slip, deformation twinning or martensitic transformation) in a continuum mechanics setting. A crucial aspect of the CP modelling is proper calibration of the parameters. This task is often carried out in an automatic fashion using various optimization techniques such as gradient optimization, Levenberg-Marquardt method, Bayesian optimization or particle swarm optimization. However, the evolutionary algorithms (EAs) seem to be the most commonly applied approach in this context. Their prevalence stems from many advantages such as easy understanding and implementation, compatibility with discontinuous objective function, good performance even when many parameters are to be optimized at the same time and ability to escape local minima. The poster presentation will first present the author's experience with EA parameter optimization of polycrystalline metals and alloys using Eshelby solution-based self-consistent mean-field models, cf. [1, 2]. Then, the recently developed optimization of CP parameters based on the results of crystal plasticity finite element method (CPFEM) simulations of instrumented indentation will be shown. In particular, the recent results will highlight the efficiency of using the minimization of the difference between load-penetration curves or surface topographies as the objective function.

References

[1] Girard, G., Frydrych, K., Kowalczyk-Gajewska, K., Martiny, M., Mercier, S., Cyclic response of electrodeposited copper films. Experiments and elastic-viscoplastic mean-field modeling, *Mech. Mater.* 153, 103685 (2021).

[2] Frydrych, K., Jarzębska, A., Virupakshi, S., Kowalczyk-Gajewska, K., Bieda, M., Chulist, R., Skorupska, M., Schell, N., Sztwiernia, K., Texture-based optimization of crystal plasticity parameters: Application to zinc and its alloy, *Metall. Mater. Trans. A* 52, 3257–3273 (2021).