UNIVERSITÄT
SIEGEN

PD Dr.-Ing. habil. B. Eidel
Heisenberg-Fellow (DFG)
Chair of Computational Mechanics
Department of Mechanical Engineering

Heisenberg-Programm
Deutsche Forschungsgemeinschaft

Crystal Plasticity Modeling of Ni-Based Superalloys – Numerical Analysis and Experimental Validation

• Motivation

For their high creep resistance at high temperatures Ni-based superalloys are used for single-crystalline blades in gas (aircraft/stationary) turbines. The composition of Ni-based superalloy is two-phase, one with semicoherent, ordered Ni_3Al precipitates of $L1_2$ type (γ'-phase) embedded in a Ni-matrix of fcc structure (γ-phase). Size of a single precipitate: $d_p \approx 0.4$–$0.5\,\mu$m.

Indentation with indenters of spherical as well as pyramidal shape are used to investigate the material's plastic behavior. The key questions in the present, combined experimental and simulation analyses are:

1. *Which continuum constitutive model is adequate for the two-phase material at room-temperature?*
2. *How does the indenter's geometrically non-isotropic, pyramidal shape influence the elastoplastic deformations of the single crystal? How does the indenter's azimuthal orientation influence the results? Will it break the symmetries of the crystal leading to pile-up pattern different from spherical indentation?*
3. *Which role plays the anisotropy in the elasticity law for the formation of anisotropic pile-up pattern?*

• Aspects of modelling CMSX-4 at room temperature

1. Since the two phases each exhibit single-crystalline, fcc composition, an fcc crystal plasticity model is chosen assuming purely octahedral slip.
2. Since the length scale of the material is much smaller than the characteristic length scale of the experiment, the two-phase composition can be neglected and modelled as a "homogenized" material.

• Crystal plasticity constitutive model

$$\begin{aligned}
\text{Multiplicative decomposition} \quad \mathbf{F} &= \mathbf{F}^e\,\mathbf{F}^p \\
\text{Plastic velocity gradient} \quad \mathbf{L}^p &= \dot{\mathbf{F}}^p\mathbf{F}^{p-1} = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha \mathbb{S}_0^\alpha \\
\text{Schmidt Matrix} \quad \mathbb{S}_0^\alpha &= \mathbf{s}_0^\alpha \otimes \mathbf{n}_0^\alpha \\
\text{Resolved shear stress} \quad \tau^\alpha &= \mathbb{S}_0^\alpha : \boldsymbol{\sigma} \\
\text{Shear rate} \quad \dot{\gamma}^\alpha &= \dot{\gamma}_0 \left|\frac{\tau^\alpha}{\tau_r^\alpha}\right|^{1/m} sgn(\tau^\alpha) \\
\text{Accumulated shear} \quad \gamma &= \sum_{\alpha=1}^{N} \int_0^t |\dot{\gamma}^\alpha|\,dt \\
\text{Hardening rate} \quad \dot{\tau}_r^\alpha &= \sum_{\beta=1}^{N} h^{\alpha\beta} |\gamma^\beta| \\
\text{Hardening coefficients} \quad h^{\alpha\beta} &= h[q + (1-q)\delta^{\alpha\beta}] \\
h &= h_0\, sech^2 \left|\frac{h_0\,\gamma}{\tau_s - \tau_0}\right|
\end{aligned}$$

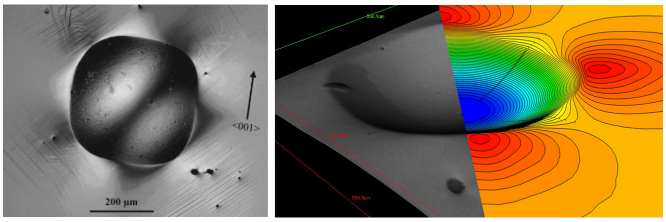

Fig. 1. : Spherical indentation into (001) CMSX-4. Left: Micrograph from experiment. Right: Perspective view on the indentation crater in experiment (left part) and simulation (right part), where pile-up hillocks emerge in <110> directions.

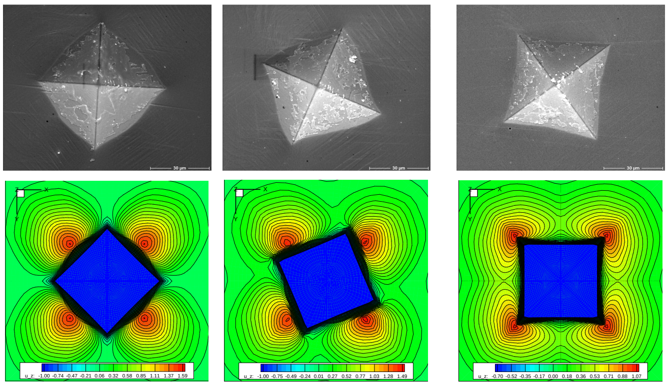

Fig. 2. : Pyramidal indentation into (001) CMSX-4. 1st row: experiment (SEM) for azimuthal orientation angle $\phi = 0°$, $22.5°$, $45°$. 2nd row: Corresponding pile-up in simulations, u_z [μm].

• Conclusions

(**I**) The pyramidal indents constantly reflect the material's cubic symmetry. Pile-up patterns invariantly emerge in <110> directions for different azimuthal orientations. The curved boundaries of the indent's rim stem from a local adaption of the indenter to the pile-up.

(**II**) Experiment and simulation show that pile-up is induced by glide on {111}<110> slip systems. It is mainly the geometry of the slip systems in the (001) oriented crystal which governs pile-up. Stress concentrations introduced by **(i)** different indenter shapes, by **(ii)** the azimuthal orientation of a pyramidal indenter and also by **(iii)** the type of the elasticity law, have minor influence.

(**III**) The "homogenized" modeling of the heterogeneous 2-phase material is adequate since accurate; it correctly predicts in FEA the pile-up pattern formation.

References

[1] Y. Wang, D. Raabe, D., C. Klüber, F. Roters, *Acta Mater.* 52 (2004).
[2] B. Eidel, PhD Thesis TU Darmstadt (Shaker, Aachen, 2005).
[3] B. Eidel, F. Gruttmann, *Comp. Mat. Sci.* 39 (2007).
[4] B. Eidel, *Acta Mater.* 59 (2011).

B. Eidel
University of Siegen, Chair of Computational Mechanics
University of Duisburg-Essen, Institute of Mechanics