Dislocation Dynamics Simulations of Mechanical Properties of Micro-Mechanical Components

D. Weygand, J. Senger, C. Motz, O. Kraft, P. Gumbsch

Plastic flow in micro-samples shows intriguing properties, such as a strong size effect – increasing flow stress with decreasing characteristic length scale of the sample – and also statistical fluctuations in the observed flow stresses at a given reference deformation and strain bursts with characteristic distributions. In the last two years, new insight into the origin of these observations has been gained using a discrete dislocation dynamics (DDD) tool developed at izbs. Our DDD tool is continuously improved, to handle more realistic micro-structures and boundary conditions. The first steps for the extension of the model to bcc materials, relevant for fusion and fission applications, have been done within an EFDA (European Fusion Development Agency) project and within a collaboration with the Paul Scherrer Institute, Switzerland (M. Samaras, W. Hoffelner).

Size effect and its micro structural origin

Micro-Pillar: The deformation behavior of single crystalline pillars with elastic properties of aluminum under nominally uniaxial load was investigated using dislocation dynamics simulations. Samples with a characteristic side length between 0.5 and 2 µm and a length to width ration of 1:2 were studied. The initial dislocation microstructure consisted of a random Frank Read source distribution (source length ~ 220nm: initial density: $2 10^{13}$ 1/m²). A summary of the flow stress at 0

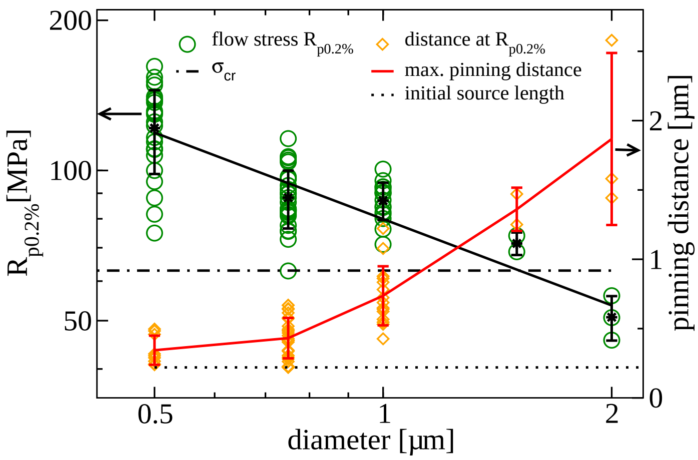

Fig. 1: Flow stresses at 0.2% plastic deformation to the left and dislocation length, characteristic for the weakest structure to the right (Scripta Mater. 2008; Mat Sci Eng A. 2008)

A clear size effect is observed within the simulations with a scaling exponent of -0.6 for the flow stress. A characteristic length for the dislocation microstructure, named “pinning distance”, is also plotted vs. the sample width *d*. This pinning distance is given by the distance between two endpoints of a mobile dislocation, where one of the endpoints has to be within the volume. It is observed that this quantity increases with increasing diameter which indicates that dislocation multiplication mechanisms are effective within the larger volumes. The flow stresses for the larger volumes are lower than the critical activation stress of an isolated Frank Read source, a value which is indicated by the dash-dotted line. For samples smaller than 1µm flow stresses exceeding the critical stress of the corresponding isolated FR sources are observed. This is due to two effects: (i) dislocation reactions may block initially mobile dislocations; and (ii) statistical effects – the probability of a favorably oriented source decreases with decreasing volume. This transition depends on the dislocation density: increasing the dislocation density reduces the transition length.

Micro-bending: The dislocation microstructure under bending shows the formation of pile-ups, a main characteristic, where the leading dislocation of a pile-up is pushed across the neutral axis and held back due to the imposed stress gradient. Back stresses will shut down the Frank Read source, and only sources close to the surface can operate multiple times. For the normalized bending moment, a power law scaling with an exponent of -0.9 beam thickness is observed. This agrees with the experimental values (C. Motz, et. al., Acta Mater. 2008).

Statistical analysis of strain bursts: Dislocation motion leads to strain bursts in micro-samples. The statistical nature of these bursts, which are localized plastic slip events, might present intrinsic limits in the formation of small scale structures. The experimentally observed burst can be described by a probability distribution following a power law with an exponent of -1.5 for the normalized burst size s. Strain bursts in discrete dislocation dynamics simulations under strain and stress control have been analyzed statistically. It was found that the simulated strain burst follows a truncated power law probability distribution with an exponent of -1.5. Fig 2 shows that strain bursts under load control extend to larger sizes whereas strain control leads to immediate relaxation. With appropriate scaling, all the distributions collapse on a master curve. The cut-off towards large burst sizes indicate that strain bursts is only visible and relevant at the microscale (F.F. Csikor et. al., Science 2007).

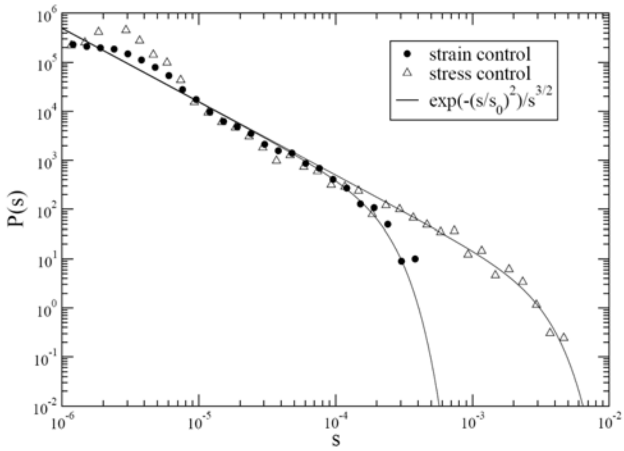

Fig. 2: Strain burst distribution for stress and strain control; s is a measure for the strain burst size and P(s) is the probability of occurrence