Simulation of a tensile test on a thin film by means of a continuum dislocation-based model

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Introduction

Plastic deformation on the microscale shows a size effect ("smaller is stronger"). There are several approaches to explain this phenonmenon. The present model was proposed by Sedláček and Werner (Phil. Mag. 83, (2003) 3735). It ascribes the size effects to the bowing of dislocations in the small samples. A continuous distribution of dislocations within a rigorous continuum-mechanics framework is considered. Our goal is to simulate a strain-controlled tensile test on thin Cu-films, and to compare the results with experiments of Hommel and Kraft (Acta Mater. 49 (2001) 3935).

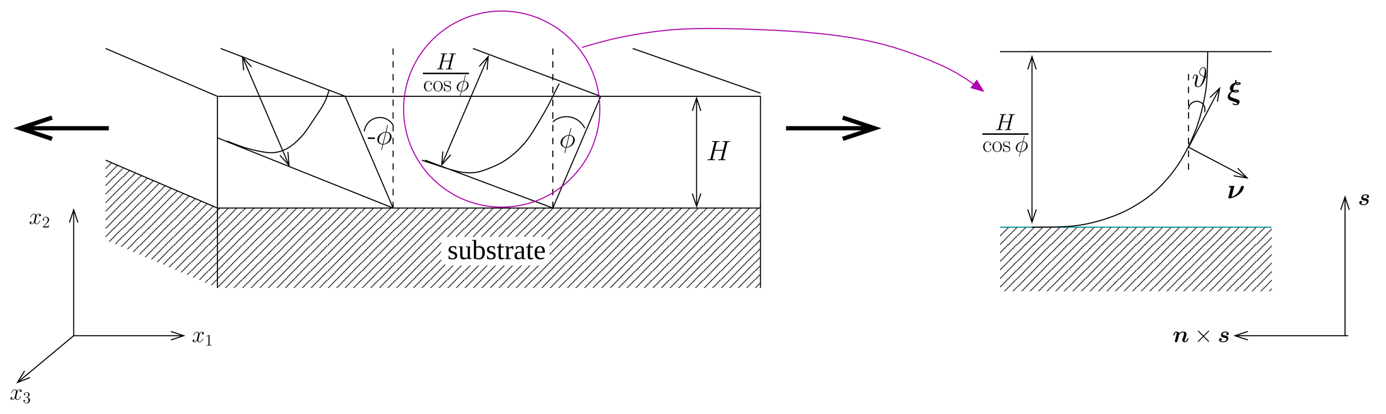
On the applied model

Fundamentals

The model is based on well established physical principles such as curved dislocations, the scalar dislocation density, the dependence of macroscopic deformation and plastic slip and the existence of a slip resistance opposing the resolved shear stress. Glide of continuously distributed dislocations in two symmetrically oriented slip systems is considered. The coupling of the dislocation model to the continuum-mechanics framework is accomplished by the standard additive decomposition of the distortion tensor. With $\boldsymbol{s}^{(i)}$ slip direction in slip system i, $\boldsymbol{n}^{(i)}$ slip plane normal, that is $\nabla \mathbf{u} = \boldsymbol{\beta}^{\mathrm{e}} + \boldsymbol{\beta}^{\mathrm{p}} = \boldsymbol{\beta}^{\mathrm{e}} + \sum_{i=1}^{m} \gamma^{\mathrm{p}\,(i)} \boldsymbol{s}^{(i)} \otimes \boldsymbol{n}^{(i)}$, here with $m = 2$.

Loading conditions

The model describes an unpassivated thin single crystalline film of thickness H on an elastic substrate that is subjected to uniaxial tension in x_1-direction. The load direction thus lies in the film plane. The plane strain approximation is adopted. By assuming homogeneity in x_1 and x_3 directions the problem becomes one-dimensional. The substrate enters the model by providing an impenetrable interface for the glide dislocations.



Model equations

Evolution equations for a representative dislocation line are set up.

- The balance equation of motion accounts for the Peach-Koehler and dislocation self force

$$Bv = (\tau - \hat{\tau})b + T\kappa,$$

B is a drag coefficient, v the slip velocity, τ the resolved shear stress, $\hat{\tau}$ the slip resistance and $T := Gb^2$ an approximation to the line tension. G denotes the shear modulus.

- The curvature κ results from the Frenet formulas as $\kappa = -\mathrm{div}\,\boldsymbol{\nu}$.
- Based upon the compatibility condition $\mathrm{div}\boldsymbol{\varrho} = 0$ for the dislocation density an evolution equation for the orientation of the dislocation line $\vartheta = \sphericalangle(\boldsymbol{\xi}, \boldsymbol{s})$ can be formulated:

$$\partial_t \vartheta = \partial_{\boldsymbol{\xi}} v - v\,\mathrm{div}\boldsymbol{\xi}.$$

- The evolution of the plastic slip is given by Orowan's equation: $\partial_t \gamma^{\mathrm{p}} = b\varrho v$.
- Additional boundary condtions are prescribed:

$$\kappa(x_2 = 0) = [Bv - (\tau - \hat{\tau})b]/T \quad \text{at the interface, such that } v(x_2 = 0) = 0,$$

$$\vartheta(x_2 = H) = 0 \quad \text{at the free surface, accounting for image forces.}$$

Modelling of hardening

Two alternative hardening models were implemented:

Model 1 The number of dislocations per unit length of the film, $\bar{\varrho}$, is held constant. The elongation of the dislocation lines due to the bowing is accounted for: $\varrho = \bar{\varrho}/\cos\vartheta$.

Model 2 The number of dislocations per unit length of the film slowly increases from $\varrho_0 = 10^{13}\,\mathrm{m}^{-2}$ to $\bar{\varrho}$. The elongation is considered as in model 1. This is the more realistic approach.

The slip resistance is approximated as $\hat{\tau} = \alpha G b \sqrt{\bar{\varrho}}$ with $\alpha = 0.6$ according to Hommel and Kraft (Acta Mater. 49 (2001) 3935).

Experimental observations

Hommel and Kraft (Acta Mater. 49 (2001) 3935) performed tensile tests on Cu-films with varying thicknesses (0.4 to 3.2 μm), grain size (0.4 to 1.2 μm) and orientation of the grains. Both sets of grains with a $\{100\}$-plane and with a $\{111\}$-plane coinciding with the film plane were examined. The tensile direction was aligned parallel to a $\langle 001\rangle$ and a $\langle 211\rangle$ direction, respectively.
The expected size dependence of the flow stress could be observed. Fitting of several established models produced results in agreement with measured trends. But none of the models can explain the big difference between the results observed for differently oriented grains and the saturation of the stress for plastic strain greater than 0.5%.

Simulation

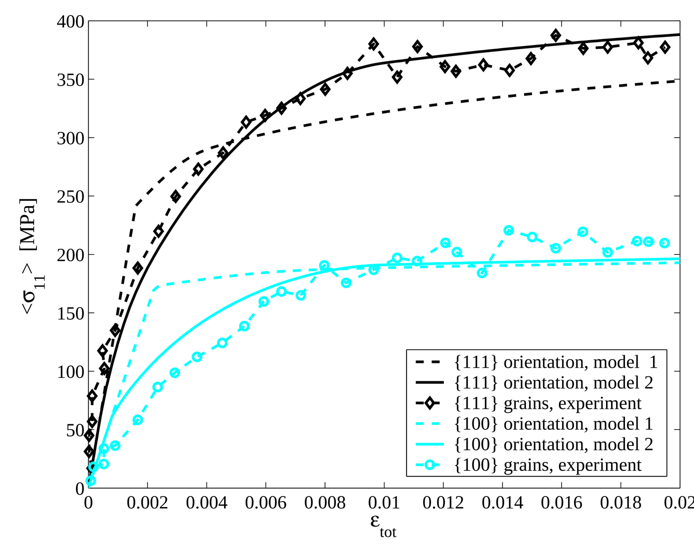
Details of the simulation

We simulate the behavior of both grain orientations separately, each as an isotropic single crystal with two active slip planes, symmetrically arranged with respect to the slip plane normal. Anisotropy of the copper film is accounted for by choosing different shear moduli G for the different orientations. The appropriate values were determined based upon results of Hearmon (Acta. Cryst. 10 (1956) 121). The initial dislocation density $\bar{\varrho}$ was chosen to get an appropriate value of the slip resistance $\hat{\tau}$, but is in the order of magnitude measured by Hommel and Kraft.

Paramter values:
$\{111\}$-orientation:
$G = 49.2$ GPa, $\phi = 19.5°$, $\bar{\varrho} = 10^{14}\,\mathrm{m}^{-2}$
$\{100\}$-orientation:
$G = 25$ GPa, $\phi = 35.3°$, $\bar{\varrho} = 4.5 \cdot 10^{14}\,\mathrm{m}^{-2}$, and for both orientations $b = 2.56 \cdot 10^{-10}$ m, $\nu = 0.35$. We interpret the necessity of a higher value for $\{100\}$-grains as expression for more dislocation interactions. The initial configuration for the computation are straight dislocation lines from the interface to the free surface, i.e. $\gamma(0, x_2) = \vartheta(0, x_2) = 0$ ('threading dislocations').

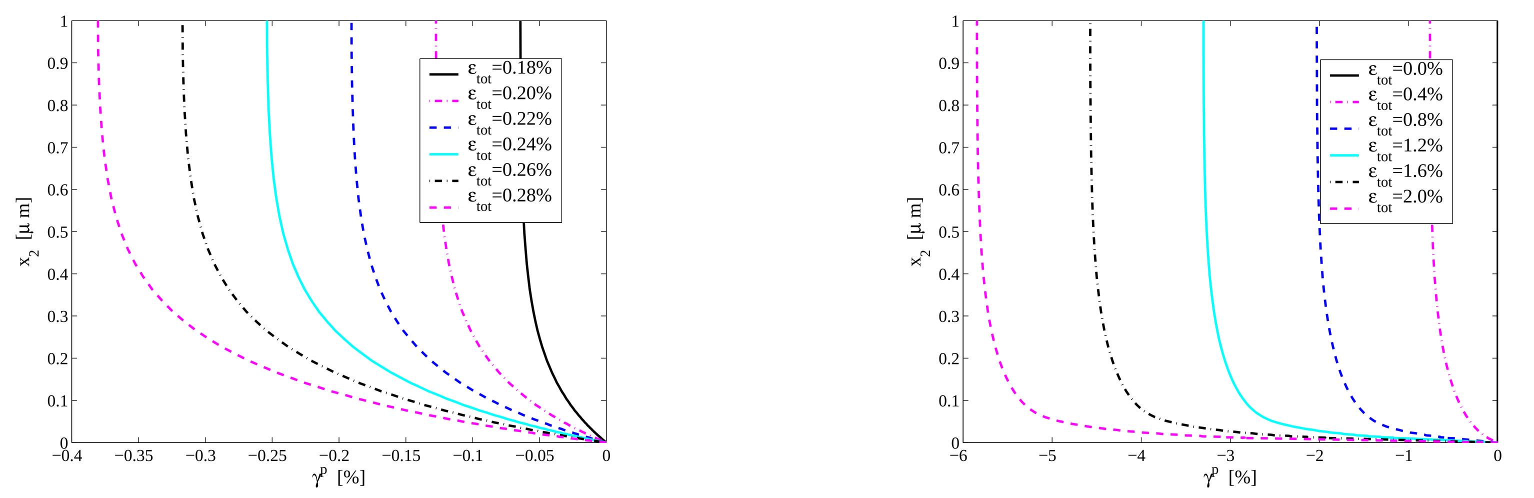
Stress-strain diagram

Comparing measured and predicted stress-strain curves, a good quantitative accordance is found. The two hardening models differ remarkably. The difference of the results for the different grain orientations is well reproduced. Apart from the influence of the orientation on the resolved shear stress in the present model the inclination angle ϕ determines the physical dimension of the slip plane, resulting as $H/\cos\phi$. The dislocations have to bow out stronger in more narrow planes, that is in planes with smaller inclination angles $\phi \Rightarrow$ higher flow stress.



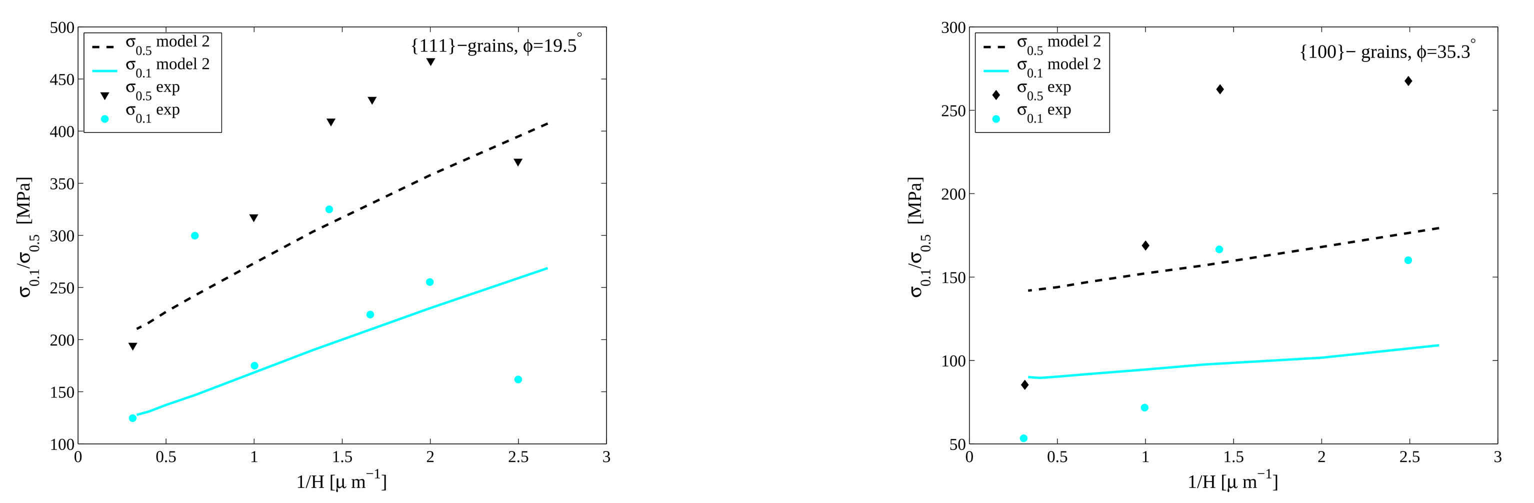
Plastic slip response

Distribution of plastic slip in the slip plane corresponds to the shape of dislocation lines. The two figures show snapshots of the glide of the dislocation in a $\{111\}$-oriented film of thickness $H = 1\mu\mathrm{m}$ under increasing deformation. For small deformations (left), the dislocation line has not yet approached the interface between film and substrate. With increasing strain (right), the dislocations bow out stronger and misfit dislocations are deposited at the interface.



Size dependence of the yield stress

There is a special interest in the explanation of the size effect. Hommel and Kraft investigated the yield stress for 0.1% and 0.5% plastic deformation as a function of film thickness. The measured values do not show a definite tendency. However, the data predicted by the simulation give a good mean approximation to them for both grain orientations.



Conclusions & Outlook

Based on well established physical principles, the investigated model is able to simulate the size effect, the dependence on orientation and the stress-saturation. In the model, the reason for the size effect is the collective behaviour of the bowing dislocations in the continuum-mechanics framework. In the future we intend to incorporate mechanisms like dislocation interactions, climbing, cross-gliding etc. in the model, and to develop a numerically and physically stable two-dimensional implementation, so that more complicated experiments can be simulated.