Continuum modelling of dislocation patterning

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Objective
The aim of the project is to model fatigue crack initiation in structural elements by taking into account the underlying processes at the mesolevel, i.e. dislocation structure development.

Motivation
Experiments show that fatigue cracks are initiated as intrusions and extrusions at the end of Persistent Slip Bands (PSBs). These intrusions and extrusions appear as a result of a different amount of net slip on glide planes within the PSB (Figure 1). It is crucial to model the development of PSBs and the dislocation structures associated to them in order to predict fatigue damage initiation.

Continuum modelling. Single slip
A single slip model based on a phase-field like approach is proposed. In the model the stress \( \sigma \) due to the presence of dislocations (as well as due to external loading) can be computed from the equilibrium equation by taking into account the plastic slip distribution \( \gamma \) in the slip system and proper kinematic and/or static boundary conditions.

\[
\nabla \cdot \sigma = 0, \\
\sigma = 4C : \left( \nabla \bar{u} - \gamma \bar{e}_2 \bar{e}_1 \right).
\]

The evolution of plastic slip is governed by the motion of dislocations under the influence of the stress field \( \sigma \):

\[
\dot{\gamma} = \frac{b^2}{B} \left( \frac{1}{6} \left| \frac{\partial \gamma}{\partial x_1} \right| + \rho_{\text{SSD}} \right) \bar{e}_1 \cdot \bar{e}_2.
\]

A distinction is made between geometrically necessary dislocations (GNDs), whose density is given by \( \rho_{\text{GND}} = \frac{1}{6} \left| \frac{\partial \gamma}{\partial x_1} \right| \), and statistically stored dislocations (density \( \rho_{\text{SSD}} \)). The latter can be nucleated and annihilated according to

\[
\rho_{\text{SSD}} = \frac{1}{6} \left( \frac{1}{L_x^2} - 2b \gamma_{\text{SSD}} \right) |\gamma|.
\]

The above set of equations is solved by the finite element method. A composite problem has taken from the literature is used to show the capabilities of the model (Figure 2); two different unit cells with anti-symmetry and periodic boundary conditions have been considered. The two different geometries used for the rigid particles give rise to quite different plastic slip patterns in the aluminium matrix material. If there is a channel between the particles (left) glide is relatively easy and therefore more plastic slip occurs. If the particles obstruct glide (right) two distinct narrow slip bands develop within the sample. GNDs concentrate near vertical walls of the particles for both geometries to accommodate the rotation of the particles.

Future work
Further elaboration of the model to include mutual trapping of dislocations is required to provide hardening.

Summary
A continuum model of dislocation density evolution has been proposed and verified for a 2D case. Because of gradients in the model, the size effect can be captured.

Figure 1 Mechanism of crack initiation

Figure 2 (top to bottom) Composite samples; Plastic slip distributions and GND density fields after 0.1% of deformation for two different geometries

As the scale of the geometry – and thus the ratio of particle size and lattice spacing \( b \) – is decreased, the predicted strength increases (not shown), thus showing a definitive size effect.

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