

## Experimental and Theoretical Studies of Incompatibility and Dislocation Pile-up Stresses at Grain Boundaries Accounting for Elastic and Plastic Anisotropies

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## Abstract

The mechanical properties of metallic materials strongly depend on the dislocation behavior, such as the density, the distribution, the nucleation and the mobility of dislocations as well as the interactions between dislocations and grain boundaries (GB). The main objective of this thesis is to study the effects of elastic and plastic anisotropies on the dislocation-GB interaction considering complex properties of GBs, misorientation effects and free surfaces effects. To reach this objective, an analytical approach based on the L-E-S formalism was investigated, which provides the elastic fields of single straight dislocations and different dislocation pile-ups at GBs in anisotropic homogeneous media, half-spaces, bi- and trimaterials while possibly considering free surface effects. The tri-material configuration allows considering a non-zero thickness in the nanometer range and a specific stiffness tensor for the GB region. The configuration with two free surfaces was used to study size effects. The effects of anisotropic elasticity, crystallographic orientation, GB stiffness and free surfaces were studied in the case of a single dislocation and dislocation pile-ups in a Ni bi-crystals with image forces and pile-ups length analyses, respectively. In parallel, in-situ compression tests on micron-sized Ni and α-Brass bi-crystals produced from FIB machining and observations coupling SEM, AFM and EBSD were performed. The compression test was performed with a low strain until slip lines were observed or yield stress was reached. Then, step height spatial variations due to localized slip bands terminating at GB were measured by AFM to determine the Burgers vector distribution in the dislocation pile-up. This distribution was then simulated by dislocation pile-up configuration in bi-crystals with the experimentally measured parameters by considering the effect of misorientation, GB stiffness, free surfaces, incompatibility stresses and critical force. In particular, the incompatibility stresses were analyzed using CPFEM simulations and the thickness of GB was simulated using atomistic simulations with LAMMPS.

## Keywords

Bi-crystal, Grain boundary, Free surface, Anisotropic elasticity, Image force, Dislocation pileup, Micromechanical testing