Influence of superimposed normal stress on the ⟨112⟩{111} shear strength in perfect fcc crystals

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The influence of stress applied perpendicularly to slip planes during shear deformation of a crystal on the shear strength is important in many deformation processes. As an example, one can consider a nanoindentation process as a combination of shear and compressive deformations in the vicinity of an indentor. Previous studies, based on the empirical Lennard-Jones potential, suggested nearly linear dependence of the theoretical shear strength on the normal compressive loading. The aim of this study is to verify those results using an ab initio approach.

Atomistic simulations of the shear deformation in fcc metals are performed using first principles computational code based on pseudo-potentials and plane wave basis set. The fcc crystals are subjected to shear deformation in ⟨112⟩{111} slip system and special relaxation procedure guarantees that all stresses will be minimized with the exception of applied normal stress and the resolved shear stress.

Obtained dependency of the ideal shear strength on normal compressive stress seem to be almost linearly increasing for all investigated crystals. Vice versa, the shear strength decreases with increasing tensile stress acting perpendicularly to slip planes.