Ab initio study of shear strength of fcc metals: influence of normal stress

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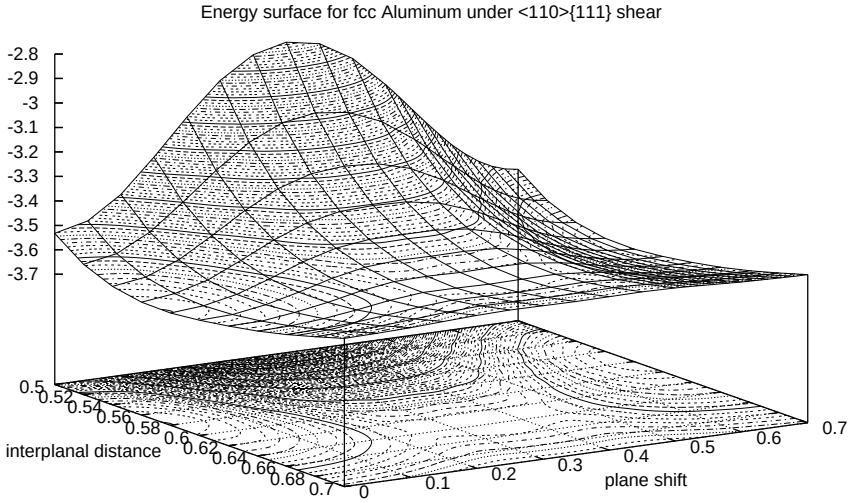
The influence of stress applied perpendicularly to a slip plane during shear deformation of crystal on shear strength is important in many deformation processes. As an example, one can consider the nanoindentation process as a combination of shear and compressive deformation in the vicinity of indentor. Previous studies [1], based on the empirical Lennard-Jones potential, suggested nearly linear dependence of the theoretical shear strength on the normal tensile and compressive loading. The aim of this study is to verify those results using ab initio approach.

Atomistic simulations of the shear deformation in fcc metals is performed using first principle method based on pseudo-potentials and plane wave basis set [2]. The fcc crystals (namely Cu and Al) are subjected to shear deformations in two common slip systems: 111<110> and 111<112>. Crystal energy is computed as a function of two independent parameters: the normalized interplanar distance (the plane distance divided by the equilibrium lattice parameter) and plane shift (see Fig. 1). The plane shift is scaled so that its values of 0 and $\sqrt{\frac{1}{2}}$ correspond to cubic (fcc) state for <110> direction and similarly values of 0 and $\sqrt{\frac{3}{2}}$ correspond to the cubic state for <112> direction. The corresponding value of normalized interplanar distance for the cubic state is $\sqrt{\frac{1}{3}}$. Such generalized γ- surface [3] allows us to evaluate both the shear and the normal stresses at any strain.



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[2] G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11169 (1996).
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