The theoretical shear strength of fcc crystals under superimposed triaxial stress

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keywords: ideal shear strength, homogeneous deformation, ab initio calculations, fcc metals

Introduction. Ab initio calculations of the theoretical strength became possible for variety of loading modes. Most of the studies were focused on simple modes where the corresponding deformation path can be described by a single parameter or where the stress state is determined by a single non-zero stress tensor component. On the contrary, materials used in majority of practical applications are usually subjected to multi-axial loading that can be also understood as a combination of several simple loading modes. From this point of view, it is possible to calculate a mutual coupling of various stresses when taking some of them as adjustable parameters and some others as the crystal lattice response.

In the present study, ab initio simulations of a uniform <112>{111} shear deformation are performed for fcc Ni, Cu, Ir and Pt crystals subjected to a superposition of shear and normal stresses. The superimposed normal stresses represent a triaxial stress state with individually adjustable components that act normally and parallel to shear planes. The main aim is to evaluate an influence of the normal stresses to TSS in a complex manner.

Computational details: The required stress state was reached applying a special relaxation procedure based on stresses computed by using first-principles pseudo-potential plane-wave code. Spin-polarized calculations enabled us to take into account the ferromagnetic ordering in Ni.

Summary: The theoretical shear strength was computed for several combinations of individually adjustable values of normal and in-plane stresses. The results revealed a variety of dependences of the shear strength on the superimposed normal and in-plane stresses for individual elements. While, in the cases of Ir and Pt, the theoretical shear strength monotonously increases (decreases) with increasing compressive (tensile) normal stress, more complex functions were predicted for Ni and Cu. All of the investigated crystals exhibited qualitatively consistent (almost linear) dependences of TSS on the isotropic (hydrostatic) stress.