Uniaxial Tensile Strength of Perfect Cubic Crystals under Superimposed Transverse Plain Stress

Miroslav Černý[a] and Jaroslav Pokluda[b]

Faculty of Mechanical Engineering, Brno University of Technology, Technicka 2, Czech Republic

[a]cerny.m@fme.vutbr.cz, [b]pokluda@fme.vutbr.cz

Keywords: stress coupling, theoretical strength, ab initio calculations.

Introduction. Most of the theoretical strength calculations were performed for simple loading modes, given by a single non-zero stress (or strain) tensor component as uniaxial or isotropic tension or simple shear. On the other hand, crystals and whiskers used in the industrial exploitation are usually subjected to multiaxial loading. Despite of this fact, just a few attention has been paid to a coupling of various stress tensor components. A typical example of rather simple multiaxial loading is a stress induced by the matrix/reinforcement incompatibility strain on the reinforcing single crystal fibre (or whisker) in a composite material. The fibres are subjected to triaxial loading even in case of the remote (purely uniaxial) tension of the composite.

This article is aimed to study the dependence of the uniaxial stress on the superimposed transverse biaxial stress for four cubic crystals. The ab initio calculation procedure was applied to Mo and W in bcc structure and Ir and Au in fcc structure. The studied crystalline systems were subjected to the uniaxial tensile stress σ_{uni} along [100] direction combined with the transverse biaxial stress σ_{bi} in the (100) plane. A relaxation procedure based on Helman-Feynman forces was applied in order to converge the stress tensor components to the state of $\sigma_1 = \sigma_{uni}$, $\sigma_2 = \sigma_3 = \sigma_{bi}$ and $\sigma_4 = \sigma_5 = \sigma_6 = 0$.

Computational details. During the relaxation process, the crystal was subjected to σ_{bi} of a certain preset value (the cell edges perpendicular to [100] direction were allowed to change their lengths in order to converge σ_{bi} to the preset value). Then the crystal was incrementally elongated in the [100] direction and the value of σ_{bi} was converged to the same preset value for any [100] strain level. The maximum of uniaxial stress σ_{max} and the related strain ε_{max} were found by a cubic spline interpolation of computed σ_{uni} values. If no other instability precedes, the σ_{max} value can be considered to be the theoretical tensile strength under corresponding superimposed biaxial stress. The relaxation procedure was repeated for several preset σ_{bi} values. The calculations of energy and stresses were preformed using a plane wave code VASP (Vienna Ab initio Simulation Package). The exchange-correlation energy was evaluated using the local density approximation (Au) and the generalized-gradient approximation (Mo, W and Ir).

Summary. Obtained results show that, within a limited range of biaxial stresses (±20 GPa), the uniaxial stress (corresponding to certain constant strain value) almost linearly increases with the increasing transverse biaxial stress. The factor that expresses the slope of the linear function changes with the applied uniaxial strain. The slope corresponding to the ultimate strain is maximal for both studied bcc crystals and minimal for both fcc crystals. The theoretical strength values for the triaxial loading corresponding to the stress state at the crack tip lie close to the value of theoretical isotropic strength.