The [100] Compressive Strength of Perfect Cubic Crystals under Superimposed Biaxial Stresses

Petr Řehák*, Miroslav Černý and Jaroslav Pokluda

Institute of Engineering Physics, Faculty of Mechanical Engineering, Brno University of Technology, Technická 2, 616 69 Brno, Czech

*yrehak02@stud.fme.vutbr.cz

Keywords: superimposed biaxial stress, tensile and compressive strength, triaxial loading, first principles calculations.

Introduction. The theoretical tensile strength (TTS) has been calculated for variety of ideal crystals and loading directions while the theoretical compressive strength (TCS) has been studied rather rarely. TCS can be calculated only for certain loading directions in particular lattices since it is usually associated with an instability dictated by a phase transition. For example, when the fcc lattice is subjected to a $\langle 100 \rangle$ loading, it acquires a tetragonal symmetry. Uniaxial compression draws the original fcc structure to the bcc one via tetragonal Bain's path. In this study, an influence of superimposed transverse biaxial stresses on the maximum $\langle 100 \rangle$ uniaxial tensile as well as compressive stresses is evaluated for Al, Cu, Ag, Ir, and Pt. A similar (triaxial) state of stress can be found, e.g., at the crack tip or in the fibre-reinforced composite materials (induced by the matrix/reinforcement incompatibility strains).

Computational details. The structure parameters were optimized to get the required superimposed biaxial stresses during the simulated compressive test by our relaxation procedure combined with first-principles computational code *Abinit*. The wave functions were represented by means of a plane-wave basis set within a pseudo-potential scheme with the Troullier-Martins pseudo-potential. The exchange-correlation part of the energy was evaluated by the Generalized Gradient Approximation for most elements except for Pt where the Local Density Approximation was used instead.

Results. Calculated TTS dependences for Ir and Pt are linearly increasing (decreasing) functions of tensile (compressive) transverse stresses in agreement with previous studies. On the other hand, the dependences for Cu, Al and Ag exhibit maxima at almost purely uniaxial loading. It was also found that all computed functions for TCS are linear with negative and remarkably higher slopes. Thus, the sensitivity of TCS to superimposed transverse stresses is significantly higher than that of TTS and its dependence is opposite for all the investigated crystals. Dependence of TTS and TCS on the transverse biaxial stresses σ_{bi} can be approximated as

$$\sigma_{max} = \sigma_r + k\,\sigma_{bi},$$

where the regression parameters σ_r and k represent interpolated values of the theoretical strength (under uniaxial loading) and the slope of the regression line (sensitivity to σ_{bi}), respectively. Note that, in the case of TCS, the result corresponds well to the behavior of real crystals containing defects, while the opposite is true for TTS.

Summary. The theoretical strength under $\langle 100 \rangle$ uniaxial compression was calculated for several constant values of the superimposed transverse biaxial stress. The results suggested that the compressive strength linearly increases (decreases) with increasing compressive (tensile) transverse stresses.