STABILITY OF FCC CRYSTALS UNDER HYDROSTATIC LOADING

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Elastic properties of perfect fcc crystals (namely, the bulk modulus, tetragonal and trigonal shear moduli and theoretical strength under isotropic tension) will be calculated via ab initio study of the energy changes under external mechanical loading.

The energy of the system will be computed by means of VASP code using projector augmented-wave potential and plane wave basis set. The exchange and correlation contribution to the total energy will be treated using generalized gradient approximation.

Several deformation paths will be taken into account. The main path conserves the cubic symmetry and changes only the crystal volume. Other deformation paths will be chosen conveniently in order to obtain required elastic moduli. The crystal energy can be expressed as a function of the Lagrangian deformation tensor as

$$E = E_0 + V\sum_i \sigma_i \eta_i + \frac{1}{2}V\sum_i\sum_j C_{ij}\ \eta_i \eta_j + O(\eta^3),$$

where V is the crystal volume, σ_i is component of a stress tensor, η_i are components of the strain tensor and C_{ij} are the elastic moduli in Voigt notation. Using this energy expansion, the elastic moduli can be calculated as

$$C_{ij} = \frac{1}{V}\frac{\partial^2 E}{\partial \eta_i \partial \eta_j}.$$

The bulk modulus $B = (C_{11}+2C_{12})/3$, tetragonal shear modulus $G = (C_{11}-C_{12})/2$ and the trigonal shear modulus C_{44} are computed for several volumes spanning from the equilibrium one up to the inflexion point of the dependence of the total energy on the volume.

In this paper, stability of the Cu, Al and Ag crystal will be assessed according to conditions originally introduced by Born and Fűrth and later modified by Hill and Milstein for a system under load. These conditions are expressed in terms of elastic constants and applied stress values. The stress, corresponding to first onset of instability is regarded to be the theoretical strength under isotropic tension.