A simple prediction of the theoretical tensile strength of cubic crystals based on the shear strength calculations

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Introduction. Uniaxial tensile tests belong to the easiest experimental strength measurements. Results of such experiments on whiskers as well as theoretical studies based on atomistic modelling of strained perfect crystals suggested that rupture of many crystals is related to reaching the shear strength in some convenient slip system rather than approaching the maximum tensile stress that leads to tearing. This work presents a simple way how to estimate the uniaxial tensile strength based on calculations of the theoretical shear strength and its dependence on superimposed normal stress.

The atomistic simulations of the shear and tensile deformations in cubic crystals were performed using first principles computational code based on pseudo-potentials and plane wave basis set. The fcc crystals are subjected to shear deformations in $\langle\bar{1}\,\bar{1}2\rangle\{111\}$ shear system and a special relaxation procedure controls the stress tensor. Taking the results obtained into account, the theoretical uniaxial tensile strength values in $\langle 111\rangle$ and $\langle 110\rangle$ directions were evaluated for selected cubic crystals.

Summary. Obtained dependence of the ideal shear strength on the normal tensile stress seems to be almost linearly decreasing function for all investigated crystals. The estimated tensile strength values in $[11\bar{1}]$ direction were found lower than the stresses necessary for tearing in most of the studied elements (except in Ir). On the other hand, the tensile stresses in [110] directions are well comparable to the corresponding tearing stresses. Considering the influence of normal stress on the shear strength reduces the tensile strength by 5–10% in case of $\langle 111\rangle$ tension and by 20–30% for $\langle 110\rangle$ tensile direction.