Selected Topics

1. Interfaces (solid/solid and solid/liquid)
2. Matter at extreme conditions / structure prediction

The theoretical strength of fcc crystals under uniaxial compression with superimposed transverse stresses

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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 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. In this work, we study the dependence of the uniaxial compressive stress (particularly its maximum value) on the superimposed transverse biaxial stress for selected cubic crystals. A necessary relaxation procedure was based on first princilpes calculations of a stress tensor. A plane-wave pseudo-potential code abinit is employed for this purpose.

The results that the compressive strength linearly increases (decreases) with increasing compressive (tensile) superimposed transverse stresses.