Shear instabilities in bcc crystals during tensile tests

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Introduction. When using various atomistic approaches, the ideal tensile strengths are often identified with maxima of calculated stress-strain curves. The considered mechanism of failure is then related to cleavage across a plane perpendicular to the loading axis. Although some of the very first tensile tests on whiskers conformed to this model, many other experiments suggested that whiskers often prefer to fail by shear on convenient shear planes. Max Born formulated conditions of crystal stability in terms of elastic constants. To apply corresponding stability analysis to a crystal under uniaxial tension is considerably more laborious approach since it requires checking the crystal stability at each strain increment. Moreover, the number of stability conditions depends on the crystal symmetry along the loading path which makes the analysis for certain loading directions (as, e.g., the $\langle 110 \rangle$ direction) extremely difficult. On the other hand, such rigorous stability analysis can yield remarkably lower values of the ideal strength (that are closer to reality) than computing the maximum axial stress.

This work presents a simple but efficient way, how to estimate shear instabilities in an ideal crystal lattice subjected to uniaxial tensile loading. The instabilities are predicted from calculated values of the theoretical shear strength (in two convenient shear systems) and its dependence on a superimposed normal stress.

Method. The atomistic simulations of coupled shear and tensile deformations in six body centered cubic crystals were performed using first principles computational code based on density functional theory within pseudo-potential approach. Selected bcc crystals were subjected to shear deformations in two shear systems ($\langle 111 \rangle\{110\}$ and $\langle 111 \rangle\{112\}$) and a special optimization procedure controlled the stress tensor to ensure that the normal stress was constant and the other stresses were relaxed (except for the shear stress) during the whole shear deformation. The obtained stress maxima were calculated for several values of the normal stress.

Summary. Computed ideal shear strength seems to be monotonically decreasing function of the normal tensile stress for most of the investigated crystals. Taking these results into account, the uniaxial tensile strength values for three crystallographic directions ($\langle 100 \rangle, \langle 110 \rangle$, and $\langle 111 \rangle$) were evaluated by assuming a collapse in the weakest shear system. The estimated strength values are, in some cases, lower than the maximum tensile stresses by more than 50%. The lowest tendency to fail by shear was observed for the $\langle 100 \rangle$ loading direction. This is in agreement with the occurrence of $\{100\}$ cleavage planes in bcc metals.

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