

Multiscale model of nanoindentation test

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The nanoindentation test in the dislocation free volume of the grain in a metallic polycrystal was simulated by utilizing a multiscale analysis. The onset of microplasticity, associated with the pop-in effect identified in experimental nanoindentation tests (generation of first dislocation loops), is assumed to be related to the moment of reaching the value of the ideal shear strength for that crystal. In particular, the influence of the compressive normal load (acting on the shear plane) on the ideal shear strength value, the three dimensionality of the nanoindentation test, the nonlinearity of the stress-strain relation, the orientation of relevant crystallographic planes and the anisotropy of elastic response of the crystal were considered in the model.

The mechanical characteristics of the perfect metallic crystal (grain) were calculated by using the ab initio approach. The three-dimensional isotropic FEM analysis was used to simulate the development of the stress-strain field in the substrate.

The computed displacement value was compared with experimentally measured pop-in effect in the nickel crystal and a good agreement was obtained. The results reveal that the nanoindentation test can serve as a sufficiently precise tool for experimental determination of the ideal shear strength.

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Section 1: Atomistic and Ab initio Simulations: Materials Properties