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Contribution of Atomistic Simulations towards Multiscale Modeling and Understanding of the Life of Defects in Crystalline Materials

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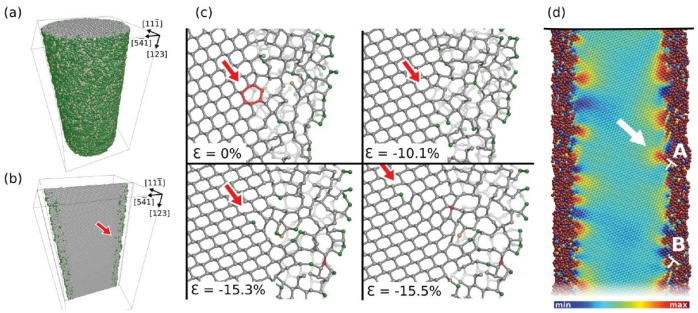
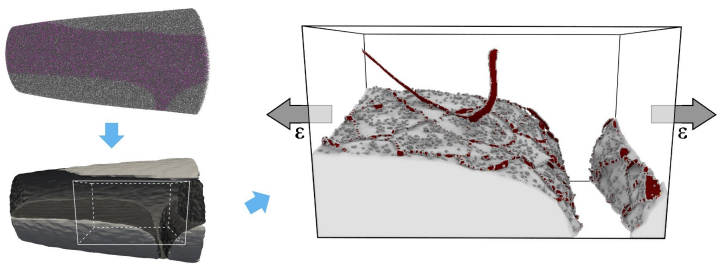
The formation, evolution, interaction, and annihilation of defects are key processes which control the behavior of crystalline materials undergoing severe structural changes, either by mechanical deformation or irradiation. These processes involve mechanisms on different scales, such as grain-boundary (GB) migration at the micro-scale, dislocation interactions at the nano-scale or point defect formation at the atomic-scale. Time aspects have also to be considered with processes being resolved in time frames of several seconds to some picoseconds. However, most of the experimental and simulation methods are limited to specific length- and time-scales. Concerted work is thus required to achieve complete understanding and accurate modeling of these processes.

Here we present the contribution of some atomistic simulations towards a multiscale understanding of the plastic deformation of crystalline materials. The dislocation absorption in GBs and the influence of internal strain on irradiation-induced damage will be shown as examples of inputs in higher scale models. The interplay of atomistic simulations and experiments will be highlighted through the initiation of plasticity in silicon nanowires, dislocation-GB interaction in metals, and the dislocation-precipitate interaction in superalloys. Moreover, the presentation of the European project ISTRESS —on the standardization of FIB-DIC procedures to evaluate the intrinsic stress at the sub-micron scale— will emphasize a close collaboration between simulations and experiments in a strong multiscale approach, from the micro- to the atomistic scale.

The focus of this presentation will be the inputs provided by these atomistic simulations to higher scale techniques and the interplay with experiments, rather than on a detailed presentation of the atomistic results.



J. Guénolé, *et al.*, Plasticity in crystalline-amorphous core-shell Si nanowires controlled by native interface defects, Physical Review B **87**, 045201 (2013).



A. Prakash, *et al.*, Atom probe informed simulations of dislocation-precipitate interactions reveal the importance of local interface curvature, Acta Materialia **92**, 33-45 (2015).