Critical intergranular cavity density for a transition from intrinsic ductility to brittleness

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Abstract

The influence of nanoscale cavities on the mechanical properties of a grain boundary is studied in a face centered cubic crystal. This first paper presents the raw data: the critical loads for emitting dislocations at a ductile crack tip and the critical loads for brittle propagation for characteristic void configurations. A first level of analysis is proposed: Pictures of the damaged zone illustrate the void growth mechanism and the time evolution of the void concentration profiles during propagation shows, in detail, the competition between growth and shear localization (Fig. 1). The use of configurational forces, to constrain the emergence of localized shear zones, enables studying dynamical cracks. It is shown that a critical void size of 5 vacancies and a density of one void every 8 a_0 along the tilt axis are necessary to observe sustained brittle cracking at the expense of plastic blunting and crack arrest.

Fracture, grain boundary, hydrogen embrittlement, Molecular Dynamics, Monte Carlo

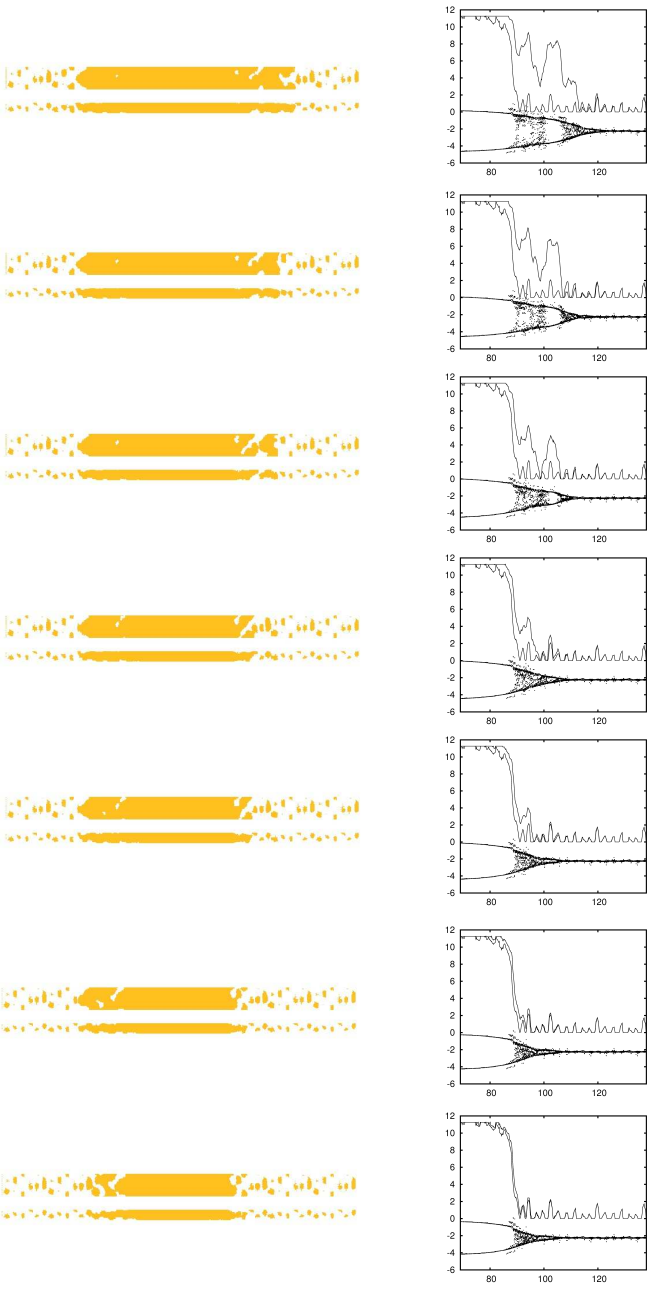

Figure 1: Sequence of pictures illustrating the truly brittle crack propagation at the critical void density: (left) top and side views of the void distributions during propagation, (right) void concentration profile and corresponding crack opening profiles.