Coupled atomistic-mesoscopic model of polycrystalline plasticity

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The description of microstructural evolution under external forces, e.g. temperature and stress, is a central subject of materials science (see e.g. [1-3]). By definition, materials microstructure comprises all the extended defects in a material (dislocations, disclinations, grain boundaries and phase boundaries, inclusions, precipitates, voids and microcracks), which can occur into different conditions as a function of temperature, stress, strain and strain-rate, and can furthermore transform into each other under the action of both the external forces and the internal driving forces. The macroscopic behavior resulting from such a complex interaction encompasses deformation, recovery and different stages of recrystallization [3]. The first level, i.e., deformation, occurring under several different experimental conditions, is the less known. Much work is yet to be done both on the experimental and on the theoretical side.

Recently [9] we proposed a *stochastic model* of microstructural evolution based on a peculiar interpretation of the Needleman-Rice variational functional P[**v**], expressed in terms of the velocity field **v** of the relevant degrees of freedom [4-8]. Our stochastic model starts from the consideration that, at the microscopic level, infinitesimal grain-boundary displacements are the result of random thermally-activated events: the probability of such events is proportional to $\exp(-\Delta H/k_B T)$ with $\Delta H = P[\mathbf{v}]\,\Delta t$, the configurational energy change (i.e., dissipation), playing the role of a transition-rate generating function. Microstructure evolution in our model thus results from a random sequence of *local*, uncorrelated events, as opposed to the *global*, (i.e, *nonlocal*) solution. We interpret the variational functional as the transition-rate generating function for the stochastic model, to be solved by means of a special implementation of the kinetic Monte Carlo (MC) method.

The two-dimensional (2-D) stochastic model above described has been subsequently extended [10] to include the anisotropy of both the grain-boundary energy and mobility, a multiphase description which allows to study, e.g., solid-liquid interfaces, the introduction of external fields such as mechanical deformation and dislocation plasticity, albeit still in a rough, oversimplified form. The microstructural model describes the evolution of the system over mesoscopic length and time scales, i.e. micrometers and seconds. However, the basic ingredients of any such model, e.g. interface mobility, bulk and interface diffusivity, interfacial energy, as well as the elementary kinetic mechanisms, e.g. boundary migration and sliding, dislocation patterning, dislocation/boundary interaction, and so on, have an *atomic-scale* origin.

In order for the mesoscopic model to be genuinely predictive, all such quantities must be generated from appropriate atomistic modelling. We have already obtained relevant results about the properties of isolated triple junctions and of their interaction in originating the *T1* and *T2* elementary events [11]. Moreover, we started the study of the interaction between isolated dislocations and symmetric-tilt grain boundaries, and crack nucleation at triple junctions [12], and the interaction between hard inclusions and microcracks [13]. Clearly, all such studies are to be understood as pieces concurring to complete the picture of the interaction among individual defects, needed to inform the mesoscopic model about the basic physics underlying.
In the present contribution we will outline the basic philosophy and some results of such a coupled atomistic-mesoscopic strategy.

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