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Development of advanced numerical algorithms for kinetic and dynamic simulations of irradiated systems : kinetic Monte Carlo and dislocation dynamics

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A novel parallel kinetic Monte Carlo (kMC) algorithm formulated on the basis of perfect time synchronicity is presented. The algorithm is intended as a generalization of the standard n-fold kMC method, and is trivially implemented in parallel architectures. In its present form, the algorithm is not rigorous in the sense that boundary conflicts are ignored. We demonstrate, however, that, in their absence, or if they were correctly accounted for, our algorithm solves the same master equation as the serial method. We test the validity and parallel performance of the method by solving several pure diffusion problems (*i.e.* with no particle interactions) with known analytical solution. We also study diffusion-reaction systems with known asymptotic behavior and find that, for large systems, boundary conflicts are negligible and do not affect the global kinetic evolution, which is seen to agree with the expected analytical behavior. We have nevertheless quantified the error incurred by ignoring boundary conflicts and discuss possible ways to make the method rigorous.

Concerning crystal plasticity, we have developed a nodal dislocation dynamics (DD) model to simulate plastic processes in crystals with low stacking fault energy where perfect dislocations split into partials, leaving a stacking fault between them. The algorithm has been applied to fcc systems. The model explicitly accounts for all slip systems and Burgers vectors observed in fcc systems, including stacking faults and partial dislocations. We derive simple conservation rules that describe all partial dislocation interactions rigorously and allow us to model and quantify cross-slip processes, the structure and strength of dislocation junctions, and the formation of fcc-specific structures such as stacking fault tetrahedra.

Vendredi 21 Mars 2008 à 10h30

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