Mechanical properties of brittle solids studied with the “learn on the fly” hybrid MD scheme.

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I will describe the main features and some initial applications of a molecular dynamics method which combines quantum mechanical embedding and classical force model optimization into a unified scheme free of the boundary region and transferability problems which these techniques, taken separately, involve.[1] The scheme is based on the idea of augmenting a classical force model by incorporating, at run time, extra quantum mechanical information necessary to ensure accurate trajectories. This is achieved through a parameter-fitting procedure in which a classical force field is adjusted “on the fly” to reproduce accurate results computed using (any number of) quantum mechanical “black box” engines.[2] The approach can be used to achieve both transferability and accuracy starting from a force model of only moderate complexity, and deals in novel ways with some traditionally difficult issues of embedding methods, such as modelling the boundaries between quantum and classical regions and ensuring energy conservation [3-6]. The scheme is useful to investigate “multi-scale” phenomena, requiring large model systems in which strongly coupled sub-regions must be modelled concurrently at different levels of precision. Test examples include point-defect diffusion and the effect of chemical impurities on dislocation diffusion. Fracture behaviour in covalent solid will be looked at in more detail. In particular, the Si(111)[1-10] crack system is found to reconstruct under uniaxial stress, predicting that a local “tip blunting” mechanism driven by elastic energy release at the crack tip region can operate in a brittle material at subcritical loads. Moreover, recent experimental observations on Si single crystals subject to [110]-oriented uniaxial tensile stress show that crack propagation is easily deflected from the (110) plane, so that novel (111) surfaces are created in a characteristic "zig-zag" crack propagation behaviour. MD simulations of model Si(110)[1-10] systems up to 200000 atoms using the SIESTA DFT code as quantum engine reveal that the effect is due to a dynamic instability in the bond breaking process, which is reached only after a crack acceleration phase. The simulations also provide a description of crack propagation as the result of a delicate interplay between dynamical stress concentration, bond-breaking and surface reconstruction phenomena taking place at the advancing crack tip region, which are at the basis of the “lattice trapping” effect in brittle materials.

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