Introduction

Atomistic simulation is a discipline based on numerically solving the fundamental equations of classical and quantum physics in order to directly predict the trajectories of the atoms which make up a physical system. That this can be done in principle has been appreciated for some time — centuries in the case of classical mechanics — but it is only with the advent of computers capable of carrying out this procedure accurately and reliably that simulation has become an indispensable research tool, complementary both to experimental and theoretical approaches. In Chapter chap:methods, I review the background to two of the main methods currently used to model physical systems at the atomic level: classical molecular dynamics and first principles quantum mechanical calculations. The former allow simulations of millions of atoms to be carried out on a nanosecond timescale Haile92,Rapaport04,Verlet67,Swope82, but the accuracy is limited by the requirement to use simple parameterisations as interatomic potentials Lennard-Jones24,SWpotential,Tersoff$_T$1, $Tersoff_T2$, $Tersoff_T3$, $Brenner90$, $Brenner00$, $Brenner02$, $Bazant97$, $Justo98$, $Marks$

In many cases we can extract enough information from these accurate quantum mechanical calculations to parametrise less transferable, but far less expensive, models as use them on a larger length scale Nieminen02. For some systems however, it is impossible to separate the behaviour on the various length scales, since the coupling between them is strong and bidirectional.

Prova

Then the only option is to carry out a hybrid simulation, where some parts of the system are treated at a higher level of accuracy Kohlhoff91,Tadmor96,Warshel76,Maseras95. An overview of existing hybrid schemes is given in Chapter chap:hybrid.

The best known example of such a multiscale system is the fracture of brittle materials, which forms the subject of Chapter chap:fracture. figure center