Modeling of crack propagation : bridge between molecular mechanics and continuum mechanics

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Context : Simulation of crack propagation is a major issue to predict the breaking of mechanical structures. Moreover, for some of these structures, it is necessary to model crack propagation at a very fine scale (nanometer scale for instance). With the increase of computing resources, simulation of crack propagation using discrete models has been performed for a decade. These models lean on features that describe materials at the nanometer scales (molecular dynamics).

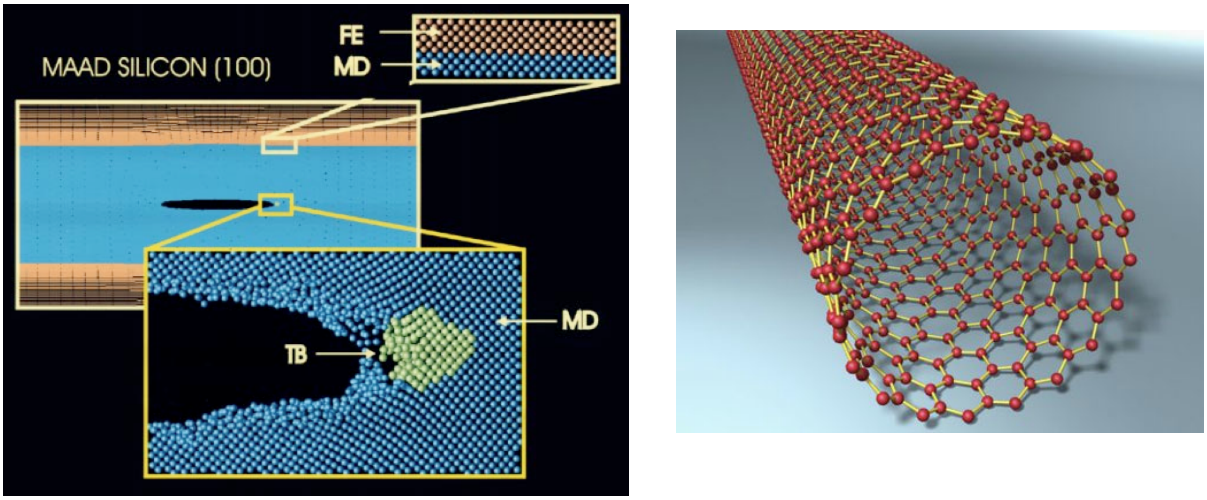

Figure 1 : Multiscale modeling of a cracked silicon sample (from Broughton et al.) and carbon nanotube

Objectives : In this work, we aim at understanding, using various numerical examples, difficulties related to the simulation of crack propagation. In particular, we will try to check whether the Griffith law, widely used in continuum mechanics, remains valid for smaller scales.

Schedule of the training:

1) Bibliography on brittle fracture;
2) Numerical aspects for crack propagation;
3) Management of the molecular statics/dynamics code;
4) Numerical study for the validity of Griffith's criterion on a graphen sheet;
5) Comparisons with results from the literature;
6) Applications for carbon nanotubes.