Atomistic Simulation Methods and their Application on Fracture

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Abstract The present work on the molecular dynamics method covers the theoretical background of the method and gives practical examples to demonstrate its capabilities and limitations. The work focusses on topics which reveal fundamental mechanisms associated with fracture processes. Moreover, promising hybrid methods based on a concurrent atomistic/continuum coupling are reviewed since they combine accuracy and efficiency in a most favorable manner.

1 Introduction

For many engineering questions connected to the mechanical properties of materials, one can of course profitably apply continuum mechanical descriptions of materials behaviour. However, when it comes to describing small specimens or when material specific questions need to be addressed, it is usually indispensable to investigate defect properties. For plastic deformation, discrete dislocation simulations (see (Kubin et al., 1992; Devincre and Roberts, 1996; Deshpande et al., 2003; Weygand et al., 2002; Weygand and Gumbsch, 2005) or the article by V. Mohles in this collection) can be applied. In these simulations the interaction of dislocation with interfaces determines the influence of the microstructures. These discrete defect based methods, however, require governing laws for the individual defect properties and more detailed descriptions for the short range interaction of defects. Such properties are difficult to obtain experimentally and are therefore usually investigated by atomistic methods.

Therefore, atomistic modelling is essential in advancing our understanding of the mechanical properties of materials. This is most obvious for the investigation of fracture processes. Materials behaviour with respect to fracture is of course ultimately determined by events on the atomic scale.
In the case of brittle fracture this connection is obvious, since the crack in a perfectly brittle material must be atomically sharp at its tip. The crack moves by breaking individual bonds between atoms and can therefore be regarded as a macroscopic probe for the atomic bonding. The transition from perfectly brittle to ductile behaviour similarly relies on atomistic processes since the multiplication or nucleation of dislocations at the crack tip is an indispensable ingredient of any modelling of the brittle to ductile transition. Atomistically the nucleation or multiplication of dislocations at the crack tip is identified with bond shearing events, which compete with the bond breaking events at crack extension.

The interaction of multiple defects, like cracks and dislocations, is still not routinely studied even with the simplest atomistic simulation methods since such studies necessarily require models that significantly extend in all three dimensions and consequently require the handling of millions of atoms. Since the application of atomistic techniques has great potential (Li et al., 2003; Kassner et al., 2005) but is still not widespread in the investigation of the mechanical properties of materials, it is probably advisable to give a short overview on the applicable methods and then to provide a few examples of successful application of atomistic modelling techniques to explain experimentally observed phenomena.

In the following section we give a general overview of the different descriptions for the atomic bonding, because they are the basis for all atomistic modelling. The next section describes the molecular dynamics method in some detail, also including the boundary conditions and visualisation of defects. This part is intended to give the reader, who is not familiar with atomistic simulation methods a feeling for the versatility of this approach. The capabilities and limitations of atomistic methods are not just related to the available description of the atomic bonding but also to the handling of boundary conditions and the analysis of the results. The subsequent section 4 deals with concurrent multiscale methods, which couple atomistic and continuum descriptions in a rather seamless manner, hence enabling the description of crystalline solids with atomistic accuracy but at smaller computational costs. The Finite Element Atomic Method (FEAt) and variants of the Quasicontinuum (QC) method are reviewed and compared.

After this methods-oriented part, in Section 5 the phenomenology of fracture is discussed in the light of atomistic modelling. First, brittle fracture is put in the spotlight, which is the domain of the atomistic methods, as we have seen above. Second, it is shown that the analysis of the plastic zone around a crack tip is now within the scope of large scale atomistic simulations.

It is noted here that this article can neither provide a practical guide