PHYSICAL MODELING OF FRACTURE MECHANICS IN COMPLEX MATERIALS

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Summary. The mechanical behaviour of brittle materials is very sensitive to microstructure defects, like point or extended lattice imperfections, elastic inclusions, voids. Since the local stress conditions (i.e. the conditions nearby a defect) of such complex materials may largely differ from their average values, the prediction of the overall mechanical response to external loads results to be a though theoretical problem. This is, for instance, the case of the stress threshold at which a microcrack starts propagating, or the interaction features bewteen the defect and the incoming crack. In this work, we investigate at the proper nanoscale the interaction between a crack tip and elastic inclusions by combining a hierarchy of different computational tools, namely atomistic simulations (carried out at the molecular dynamics level) and statistical mechanics models (based on replica-symmetry breaking). The investigated material is silicon carbide, i.e. the prototypical example of brittle material with directional and covalent bonding.

INTRODUCTION and MOTIVATIONS FOR PHYSICAL MODELING

The design of new materials for advanced applications requires a better fundamental understanding of the correlation between microstructure, elastic/plastic properties, and mechanical response. This is, in particular, the case of covalently-bonded materials where several technological applications (namely, in aerospace and nuclear industry) are affected by their fragility under external mechanical and/or thermal stresses. In fact, such materials (in this context we will mainly refer to SiC) are extremely brittle, undergoing fast fracture at low temperatures.

The complex interplay of microscopic (indeed, atomic-scale) events hidden behind the apparently simple phenomenology of brittle fracture has led in the past years to an ever increasing number of theoretical and computer-based simulation studies. Among the mechanical properties, the problems of the nucleation and the evolution (growth) of brittle cracks – which are a key issue in the design of engineering stuctures – have generated a considerable body of theoretical work. Nevertheless, there are several fundamental issues still unsolved in the modern theory of brittle fracture, both in the quasi-static and dynamic domain.

Whitin the above scenario the computer-based investigations firmly rooted in the atomistic description of the material – hereafter referred to as *physical* (or *atomistic*) *modeling* [1] – are playing an increasingly important role. For example, in modern atomic-scale studies of crack propagation all of possible behavior show, from a strictly discontinuous dynamics ("lattice trapping") characterized by a complex emission of sound waves accompanying the discontinuos crack tip velocity, to a continuous behavior with a smooth opening of the running crack.

In this work we present a typical application of such an atomistic modeling to fracture mechanics with a twofold aim: (i) we like to present and discuss both conceptual and numerical problems underlying physical modeling, and (ii) we want to investigate the specific case of the interaction between a crack tip propagating into SiC towards/against elastic inclusion(s).

Since atomistic simulations are severly limited by their huge computational workload, they cannot in fact represent the only tool for the theoretical physicist interested in fracture mechanics. As a matter of fact, they need to be hierarchically combined to higher-order models (spanning the meso-/macro-scale) like, relevant to the present case, statistical mechanics ones. We therefore develop in the second part of this work a statistical approach to connect the theoretical strenght, the aging effects on mechanical properties and the local fracture toughness randomness (and/or fluctuations). In particular, we will study the macroscopic dynamics of crack fronts in disordered media by means of a statistical mechanics approach based on the replica-symmetry breaking

ATOMISTIC SIMULATIONS

The atomistic modeling relies on the description of the investigated system as an assembly of interacting particles. The goal is to derive the mechanical properties of interest directly from the collective response of atoms to suitable external loads. According to this definition, atomistic modeling represents for fracture mechanics a fundamental theory, not requiring the definition of *ad hoc* constitutive equations and/or phenomenological parameters.

The most natural way to carry out atomistic modeling is by means of molecular dynamics (MD) simulations: the atomic trajectories of a set of interacting particles – representing the mechanical system – are generated by computer in arbitrary conditions of temperature, load, state of aggregation. As for the present investigation, MD naturally drives to the optimal atomic-scale description of those relevant phenomena occurring at the tip of a mobile crack. In fact MD can effectively model the complex bond-breaking, bond switching, and rebond events observed at the very end of a crack propagating into a covalenty-bonded material. They represent, in turn, the "elementary" events ruling fracture.

We developed an efficient MD code suitable to simulating the propagation of a fracture into an atom-resolved β-SiC lattice. The propagation of the crack has been simulated by the application of an external driving force (load),

according to the modern theory of the representation of mechanical loads within a MD simulation scheme [2]. This technique will allow for the simulation of the relevant phenomena in arbitrary conditions of temperature and/or stress.
Our results provide a thorough analysis of the interaction feature between a crack tip and an elastic inclusion, either harder (diamond-like) or softer (silicon-like or void) than the host matix. The analysis is carried out in terms of both strain and stress fields.

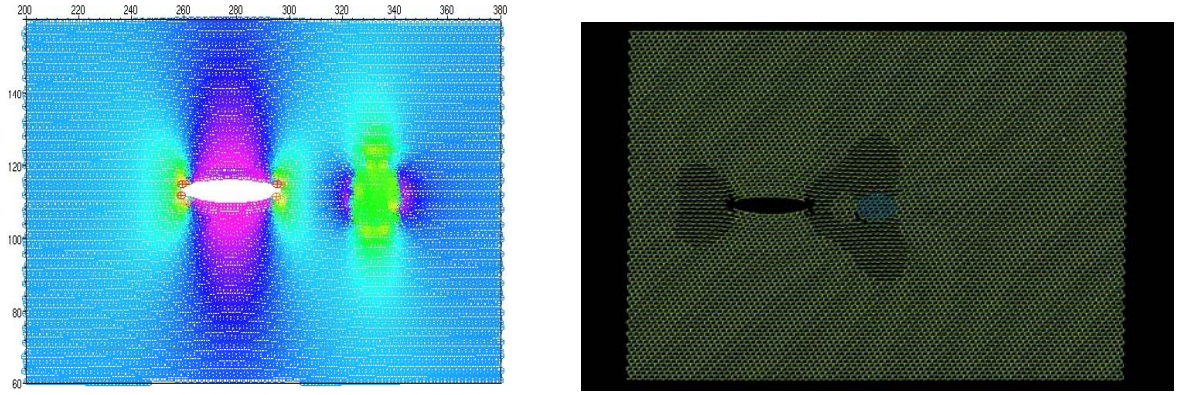

Fig.1 – *Side view for the interaction between a crack and a diamond-like inclusion in cubic SiC. A tensile load is applied normally to the pricipal crack axis. Left: total stress field (green: tensile; purple: compressive; light blue: stress conditions corresponding to the applied load). Right: similar situation now shown in terms of atomic positions and (distorted) chemical bonds. The dimensions of the computational sample are 1nm×47nm×36nm, corresponding to 155520 particles in the simulation cell.*

STATISTICAL MECHANICS MODELS

When considering more complex situations like, for instance, the roughening of a crack front during a fracture event, a straightforward atomistic simulation is simply impossible because of computer limitations. In this case we need to implement mesoscopic models based on statistical mechanics which, however, must still maintain some basic information about the underlaying lattice nature of the material.
We discuss a specific model developed to address the problem of a crack front propaganting in elastically disordered media. In this case, the crack front is faced to a pinning force due, in turn, to local (i.e. randomly distributed on lattice sites) fracture toughness. The elastic restoring force is therefore a result of the line tension of the crack front due to local bulk elasticity of the medium (in brittle materials). Under strong pinning conditions, it is well known that, when subjected to an external driving load, the crack front displays local instabilities that force it to advance quasistatically. This property makes it difficult to handle the problem in the continuum approximation and makes the present statistical approach worthy.
We effectively described the above problem by an extremal model: only the fracture site (which is mappend onto the lattice) closest to its instability threshold advances. After a jump, the instability thresholds of all the sites are modifed by the (elastic) couplings between sites. The proposed model belongs in fact to a wide class of extremal models which have already been studied extensively. The common feature consists in the attempt to explain driven motion under strong pinning by means of a discrete, deterministic dynamics. Only one site is active at every instant of time. Further the extremal condition can be thought of as a way to retain the information of the spatially quenched heterogeneities that determine the evolution of the front. All the information in this dynamics is clearly contained in a space-time "cracking plot", i.e. the geometriucal locus where the front is active: most of the relevant physical information will be discussed in terms of the probability density function of such a plot.

ACKNOWLEDGEMENT

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