# ATOMISTIC SIMULATIONS ON FRACTURE EVENTS IN NANOSTRUCTURED SILICON CARBIDE

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**ABSTRACT**
We present the conceptual framework of atomistic simulations applied to the investigation of mechanical properties of materials. As a show-case application, we discuss a fracture event in bulk silicon carbide when a hard nanofiber inclusion of diamond is present in the neighborhood of a microcrack. We show that, for suitable distances between the two defects, the nanofiber inhibits the propagation of a fracture event from the microcrack tip. This result is consistent with the suggestion that fiber reinforcement could provide increased fracture thoughness in ceramic materials.

## 1. INTRODUCTION

The theoretical and computational investigation of the mechanical properties of materials has been traditionally ruled out by continuum theories, among which the elasto-plastic theory has played (and in fact it is playing) the role of "standard model" (Broberg [1]). The computational counterpart of continuum modelling is represented by finite element analysis.

The technological rush towards nanometer-sized systems has forced researchers to investigate mechanical phenomena at a length scale appearing to be very challenging for continuum modelling, either conceptually and computationally. This is the case, for instance, of investigating the propagation features of a microcrack into a material displaying elastic or structural complexity at the nanoscale. Let us focus on the specific case of a microcrack propagating - provided that the Griffith instability condition is reached upon suitable loading - into a nano-composite material, where occasionally it is faced to phase boundaries between the matrix and the fiber. There are serious conceptual and computational limitations in applying continuum modelling to such a case. As a matter of fact, stress and strain fields computed by continuum theories at vanishing distances from the crack tip become mathematically singular (Broberg [1]), thus preventing any meaningful prediction of mechanical behaviour in the near vicinity of the crack tip, i.e. at the length scale where it could possibly occur a direct interaction between the crack tip and the phase boundary or inclusion. Furthermore, the corresponding total computational workload of a continuum analysis based on finite elements would result prohibitively large for an excessive refinement of the numerical mesh, as indeed necessary for systems with inhomogeneity at such a short length scale. Typically, the mesh refinement would therefore be stopped at a larger scale representing a (possibly bad) coarse grain picture of the actual nanoscale structural complexity.

In order to cope with similar problems, during the last twelve years or so a novel approach based on a direct atomistic description has emerged as a valuable conceptual as well as numerical tool for materials nanomechanics. The key-idea of atomistic modelling is to look at a solid body under mechanical load as an assembly of atoms interacting through direct coupling: their collective response to loading will eventually drive the overall mechanical response, i.e. - for the above discussed case - it will drive the propagation of the microcrack. Since the material is now resolved atomistically, there is no ambiguity in representing the actual nanostructure displaying in principle any combination (at any possible relative distance) of cracks, phase boundaries or

whatever kind of elastic inclusion. Furthermore, the mathematical singularity of stress/strain fields at the crack tip is naturally removed when mapping the problem onto a discrete atom-resolved lattice. The elementary step for crack advancement is in fact represented by a bond-breacking event, while the corresponding strain field is simply computed by the prediction of the new atomic coordinates (just after the bond snap). Accordingly, the local stress is computed on each displaced atom, so that no singular behaviour is ever reached.

The above discussion points out how atomistic modelling naturally operates at the length scale falling out-of-reach of continuum theories. In addition, since the response is represented by the collective displacement of atoms, the mechanical behaviour is here governed by the selected interatomic potentials that, in turn, are determined by a fundamental analysis of chemical bonding between atoms. In other words, the selection of suitable constitutive equations for the mechanical behaviour is no longer needed: under this respect, atomistic modelling could be viewed at as a first principles mechanical theory.

In this work we discuss a specific application of atomistic modeling, namely molecular dynamics (MD) simulations, to the investigation of the interaction between a microcrack tip and an inclusion (either hard and soft) in silicon carbide. This model system represents the case a nanofiber-reinforced ceramic material of great potential interest for aerospace applications. This paper is organized as follows: in Section 2 a brief tutorial introduction to MD simulations is offered, while in Section 3 results are presented and discussed.

## 2. THEORETICAL FRAMEWORK

The basic idea underlying molecular dynamics simulations (Frenkel and Smit [2]) consists in describing the dynamics of the investigated system – in any state of aggregation or under arbitrary loading conditions – as the collection of single-particle movements due, in turn, to interatomic interactions.

Once that a suitable interatomic potential $U(R_1,R_2,\ldots R_N)$ depending upon the coordinates $R_i$ of all of particles is known, we can easily (from the conceptual point of view) compute the force acting on each particle and, according to Newton dynamics, we can compute its trajectory. In order to do so, we need: (i) to operate a discretization of the time evolution by finite time-step increments; and (ii) to assume that interatomic forces are constant over such a time interval. The equations of motion for each particle are then solved by finite difference methods iteratively at each time-step. It is important to remark that the interatomic potential $U(R_1,R_2,\ldots R_N)$ is developed on the basis of a robust understanding of the chemical bonding and it contains, in principle, any contribution from steric, angular, and many-body particle-particle interactions. In other word, MD is a theory intrinsically containing any mechanical effect, ranging from the linear elastic to non-linear and/or non-elastic regimes.

Since the time discretization must be adapted to the very fast atomic dynamics, the typical time-step of a MD simulation is as small as $10^{-15}$ s. In practical applications this implies that the basic MD loop "*compute forces* $\rightarrow$ *update atomic positions*" must be iterated hundreds of thousands or even millions times. Any single loop requires, in turn, a possibly huge number of floating point operations to compute forces and to integrate Newton's equations. In other words, serious practical limitations exist in performing MD simulations in the realm of solid mechanics, as due to the heavy resulting computational workload which, in the most favourable cases and/or for efficient numerical implementations, increases linearly with the number N of atoms in the simulation cell. So far, most of MD simulations in this field have been limited to the nanoscale. We will do the same.

In this work we apply the above computational scheme to the investigation of some fracture events in nanostructured SiC. To this aim, we made use of the many-body interatomic potential by

Tersoff (Tersoff [3]), which is known to well reproduce the macroscopic structural, elastic, and mechanical properties of bulk silicon carbide (Tang and Yip [4]; Tang and Yip [5]). More recently, we have proved that the same potential correctly reproduces the strain and stress fields generated by either an isolated microcrack and an isolated hard inclusion in β-SiC (Mattoni et al. [6]).

## 3. RESULTS

In Fig.1 we show the total stress created by a microcrack (left) placed nearby a diamond inclusion (right). MD simulations indicate that it exists an attraction basin between the two objects. Since no bond rearrangement occurs, we can conclude that the observed minimum in the energy basin has to be attributed to the interaction between the stress fields of the microcrack and of the hard inclusion. A detailed discussion is reported elsewhere (Mattoni et al. [6]). Here we simply point out that the stress intensification at crack tips predicted by elementary elastic theory is correctly reproduced by atomistic simulations, while a complex distribution of tensile (yellow and green) and compressive (purple and blu) stress is created in the sample with respect to the uniform asymptotic stress value (light blue). The computational sample is loaded so to suffer a homogeneous 8% strain before insertion of the defects.

The question we address here is whether the interaction between the microcrack and the inclusion also affects the toughness of the sample against fracture. This question is related to the suggestion that a possible improvement toward an increased fracture thoughness in ceramic materials could be fiber reinforcement (Kuntz et al. [7]), i.e. the incorporation of suitable fibers into a ceramic matrix. To this aim, we applied a suitable loading to the system shown in Fig.1 normally to the microcrack axis, beyond the theoretical Griffth stability threshold as measured by direct MD simulations for a bulk system containing just the microcrack defect. The actual border conditions – implemented by the constant-traction MD algorithm (Cleri [8]) – correspond to the plane strain conditions of continuum mechanics.
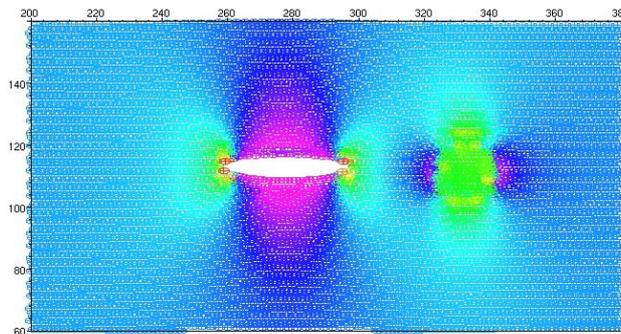


Figure 1: Total stress field created by the microcrack (left) and a diamond hard inclusion (right) in β-SiC, when placed at 5.5 nm distance and under 8% strain condition.

The results of such a loading test are shown in Fig.2. In any case we applied the same loading conditions, but we explored two relative distances between the defects, respectively 8.25 nm (right) and 5.5 nm (left). While in the first case a fracture is indeed observed propagating from the

right microcrack tip, in the second one no such event is observed indicating that fiber reinforcement effectively takes place. A direct explanation can be extracted from the snapshot pictures reported in Fig.2. Yellow sticks represent the network of Si-C bonds. Nearby the defects chemical bonds are elongated, since we are in the regions of net tensile stress (see Fig.1). However, for a large enough separation between the microcrack and the inclusion (Fig.2, left) there is no sizeable interactions between the two stressed-bond regions and the crack can indeed propagate since – as explained above – we are beyond the Griffith threshold and the microcrack behaves as an isolated defect. On the other hand, when the defects are close enough, the network of distorded bonds is completely different than the isolated microcrack case, effectively driving to a local loading conditions below the Griffith threshold.
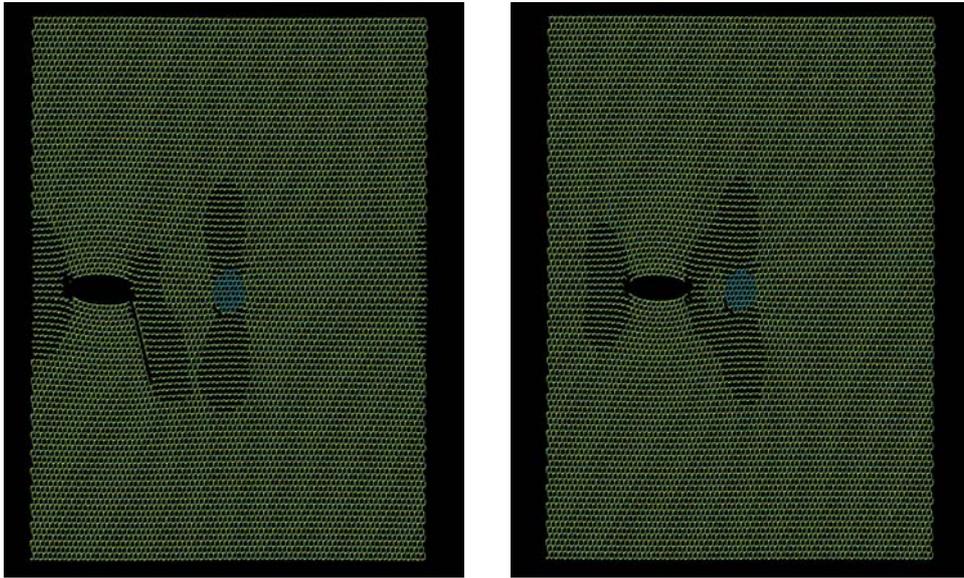


Figure 2: A microcrack is placed at 8.25 nm from an hard diamond inclusion in β-SiC (left). The system is loaded beyond the Griffith threshold and a fracture event is observed. When the relative distance is decreased down to 5.5 nm the same loading conditions cannot generate a fracture event (right).

In conclusion, we have shown that molecular dynamics simulations can be efficiently applied to the investigation of mechanical phenomena in solids, reproducing some basic results of elementary continuum theory. Furthermore, MD simulations can provide valuable physical insight on the relevant atomic-scale phenomena ruling the fracture behaviour of a nanostructured ceramic material.

## 4. REFERENCES

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