STRESS AND STRAIN FIELDS OF A CRACK-INCLUSION PAIR IN β-SiC: AN ATOMISTIC INVESTIGATION OF NONLINEARITY EFFECTS

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ABSTRACT

We investigate the interaction of a microcrack and an inclusion in monocrystal β-SiC under plane strain loading condition. By means of molecular dynamics simulations we are able to represent properly the mechanical loads and to calculate the stress and strain fields when the distance of the microcrack and the inclusion is varied. When the crack-inclusion distance is large respect to the dimension of the isolated defects our results are consistent with the basic results of the linear elastic fracture mechanics, and provide a deeper insight at the nanoscale. At small crack-inclusion distances the stress and strain fields are not additive respect to the isolated microcrack and inclusion and we calculate such a defect of linearity. We find power law dependence of the stress and strain defect of linearity on the relative distance of the microcrack and the inclusion.

1 INTRODUCTION

Silicon carbide, as other ceramic materials, is attractive because of its physical and chemical properties such as high hardness, low density and high inertness. Nonetheless its structural applications still remain limited due to brittleness and low fracture thoughness.

It has been proposed that the macroscopic fracture toughness may be increased by introducing in the ceramic matrix a distribution of hard fibers (fiber toughening). Toughening is the macroscopic result of complex mechanisms, such as crack deflection or fiber bridging (Kuntz [1]). It is clear that the core problem is the interaction of the crack tip and the inclusion. According to the Linear Elastic Fracture Mechanics (LEFM), the stress at the crack tip is enhanced with respect to the remote loading value. The failure of the system is related to such stress intensification at the crack tip. When an inclusion is introduced into the system, the stress field at the crack tip is affected and the previous picture has to be accordingly modified. A detailed understanding at the nanoscale of such effect is relevant to control the structural stability of the system and it is still missing.

Molecular dynamics (MD) is a well established computational tool in materials science (Frenkel and Smit [2]). Once a reliable model for the interatomic forces is given, several physical properties may be investigated by MD. Recently MD simulations have been successfully applied to study the nanomechanics of crystalline, non-crystalline, brittle, and plastic materials. Nanomechanics requires some methodological improvements respect to standard MD simulations to properly represent the loading condition at the nanoscale and to find a suitable definition of local stress and strain fields.

Here we present an atomistic analysis of the interaction between a nanosized microcrack and an inclusion in monocrystal β-SiC considering both the case of hard and soft inclusion. We consider the diamond fiber as prototype of hard inclusion and silicon fiber as a prototype of soft inclusion. Hard inclusions have been chosen to be coherent respect to the matrix lattice structure. In fact it has been experimentally proved that coherent diamond inclusions with size of about 3 nm

may form in monocrystal β-SiC by carbon implantation (Pecz [3]). We focus our investigation to parallel alignment between the two defects and consider extensively the case of stable microcrack.

Such analysis is performed by studying the stress and strain fields of a crack-inclusion pair and calculating the effect of the inclusion on the crack-induced stress field. Furthermore we explore the nonlinearity of the total stress field respect to the case of isolated microcrack and inclusion. Nonlinear correction to the stress field may be relevant close to the threshold of microcrack stability and are investigated in detail as a function of the distance between the defect.

2 ATOMISTIC DESCRIPTION OF STRESS AND MECHANICAL LOAD

The typical simulation cell is represented in Fig. 1 and it consists in a thin slab containing 60480 atoms of monocrystal SiC with zincblend structure (β-SiC). The x, y and z axis were aligned along the [11-2], [-110] and [111] orthogonal directions, respectively. In the z direction the system was elongated in steps up to a tensile strain of 8% by means of the constant traction method (Cleri [4]). In the x-y plane the system was kept at the equilibrium lattice parameter of β-SiC and periodically repeated.

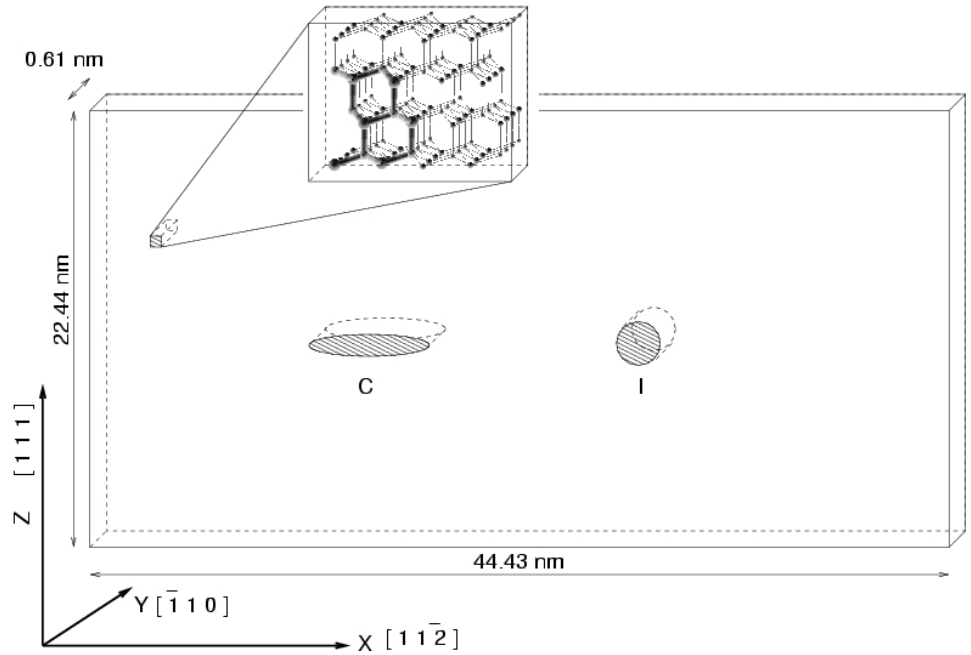

Figure 1: Geometry, orientation, crystal structure, and dimension of the simulation cell. Both the microcrack (C) and the cylindrical inclusion (I) are shown as well.

This geometry corresponds to the plane strain border conditions of continuum mechanics. Molecular dynamics simulations are based on Tersoff potential (Tersoff [5]) that properly describes thermomechanical properties of β-SiC (Tang [6]). Furthermore, the Tersoff potential is able to reproduce the brittle failure of silicon carbide under tensile load.

The stress tensor $\sigma_{\alpha\beta}$ of a system at T=0 K is in principle defined as: $\sigma_{\alpha\beta}=V^{-1}dU/d\varepsilon_{ab}$ where U is the internal energy of the system and ε_{ab} is the strain tensor for the cartesian coordinates α and β. Within the Tersoff force model it is possible to cast the energy U of the system into a sum of single-site energies ν_i; namely $U=\Sigma_i\nu_i$. Similarly we get an expression for the tensor $\sigma_{\alpha\beta}$ in

terms of atomic stresses $\sigma_{\alpha\beta,i}$ once we attribute to any atom the same volume. For any pair i-j interacting atoms we calculate the average atomic stress $\frac{1}{2}(\sigma_{\alpha\beta,i}+\sigma_{\alpha\beta,j})$ and we attribute it to the average atomic position of the selected i-j pair. Accordingly to the plane strain border condition the dependence of stress and strain fields on y direction may be ignored and as a result we calculate the stress tensor $\sigma_{\alpha\beta}(x,z)$ in the x-z plane. Further details about the method and atomistic definition of stress may be found elsewhere (Mattoni [7]).

To validate present definition of local stress let us consider the case of an isolated and stable (111) microcrack of semi-length a =1.8 nm and center (x_C,z_C). The microcrack was obtained by cutting a number of bonds accross a shuffle plane (111) in strained β-SiC (at 8% of tensile stress). In response to the applied load the microcrack turns into an elliptical Griffith-like hole (Griffith [8]).

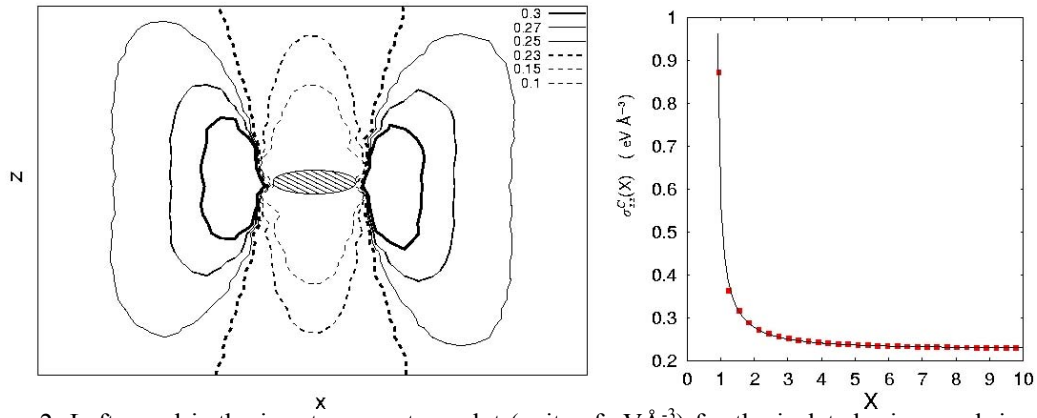

Figure 2: Left panel is the iso-stress contour plot (units of eVÅ^{-3}) for the isolated microcrack in strained β-SiC (8%). Only a 14 nm × 8 nm large portion of the system is represented. Right panel represents the stress component $\sigma_{zz}^{C}(X)$ as a function of the distance in reduced units ($X= (x-x_C)/a$) from the crack tip.

In Fig. 2 (left panel) a contour map of the stress is represented in the x - z plane showing the formation of two tensile lobes that extends outwards from the crack tips in agreement with the stress enhancement at the crack tips predicted by elementary models of fracture mechanics (Broberg [9]). The agreement is also quantitative; in the right panel of Fig. 2 the stress component $\sigma_{zz}^{C}(X)$ calculated along a horizonal line from the right crack tip has been fitted by the analytical stress curve of the Inglis model (Broberg [6]).

The diamond inclusion was obtained by selecting a cylindrical region with axis parallel to y direction, center (x_I,z_I) and radius R=1 nm and replacing its silicon atoms with the same number of carbon atoms. No defects formed at the interface matrix/diamond in agreement with experiments.

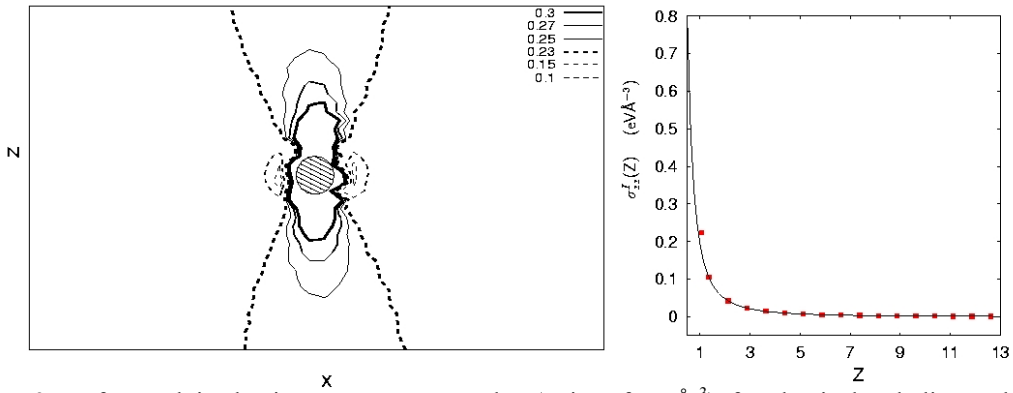

Figure 3: Left panel is the iso-stress contour plot (units of eVÅ^{-3}) for the isolated diamond inclusion in strained β-SiC (8%). Only a 14 nm × 8 nm large portion of the system is represented. Right panel represents the stress component $\sigma_{zz}^{I}(Z)$ as a function of the distance in reduced units $Z=(z-z_I)/R$ from the inclusion in unstrained β-SiC.

A map of the stress $\sigma_{zz}^{I}(x,z)$ for strained β-SiC (8%) is represented in Fig. 3 (left panel). The C-C bonds are smaller than the SiC bonds and pull them in the [111] direction; as a result two tensile lobes form along the z direction. In the right panel of Fig. 3 we plot the zz stress component $\sigma_{zz}^{I}(Z)$ calculated along a vertical line starting at the center of the inclusion in the case of unstrained β-SiC. Data are well fitted by the $1/z^2$ asymptotic behavior predicted by the continuum elasticity (Eshelby [10]).

3 INTERACTION BETWEEN THE MICROCRACK AND THE HARD INCLUSION

The map of stress for strained β-SiC (ε_{zz}=8%) when the microcrack and the inclusion are both present in monocrystal β-SiC is represented in the left panel of Fig. 4. The relative distance is 5.5 nm. The lobe of the highest tensile stress at the right tip of the microcrack is made smaller by the compressive lobe of the inclusion. In other words tensile and compressive stress tend to compensate and the β-SiC matrix turns out to be toughened by the diamond fiber. Let $\sigma_{zz}^{CI}(x)$ be the stress calculated along a horizontal line when both the defects are present. The line is chosen to pass through the defect centers. We name it total stress for the crack-inclusion (CI) pair and we represent it in the right panel of Fig. 4. We can compare the total stress with that one calculated in a system containing just one microcrack or just one inclusion at the same strain and accordingly define Defect Of Linearity (DOL) of the zz component of the stress:

$$\sigma_{nl}^{CI}(x) = [\sigma_{zz}^{CI}(x) - \sigma_{zz}^{\infty}] - [\sigma_{zz}^{C}(x) - \sigma_{zz}^{\infty}] - [\sigma_{zz}^{I}(x) - \sigma_{zz}^{\infty}] \quad (1)$$

where σ_{zz}^{∞} is the uniform stress background due to the external load. According to the present atomistic simulations, $\sigma_{nl}^{CI}(x)$ turns out to depend on the relative distance between the defects. If we rescale profiles corresponding to different distances so that the height of the peaks at the right

crack tip are the same we find the result reported in right panel of Fig. 5.

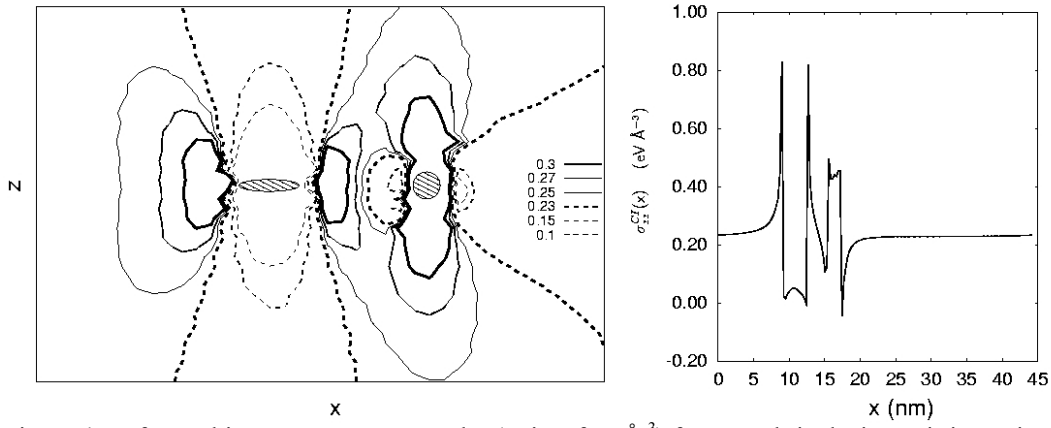

Figure 4: Left panel is Iso-stress contour plot (units of eVÅ^{-3}) for a crack-inclusion pair in strained β-SiC (ε_{zz} =8%). Only a 18 nm × 10 nm large region of the system is represented. Right panel represents zz component of the total stress $\sigma_{zz}^{CI}(x)$ showing the stress intensification at the crack tips.

We can conclude that, once rescaled, the DOL's corresponding to different relative CI distances are qualitatively similar. Furthermore the behaviour of DOL of the stress is represented by a function vanishing everywhere, but for two rather localized regions corresponding to the positions of the microcrack and the inclusion. We can extend our analysis to the strain field as well. Introducing now the DOL of zx component of strain $\varepsilon_{nl}^{CI}(x)$

$$\varepsilon_{nl}^{CI}(x) = [\varepsilon_{zz}^{CI}(x) - \varepsilon_{zz}^{\infty}] - [\varepsilon_{zz}^{C}(x) - \varepsilon_{zz}^{\infty}] - [\varepsilon_{zz}^{I}(x) - \varepsilon_{zz}^{\infty}] \quad (2)$$

we get the result shown in the left panel of Fig. 5, corresponding to four different relative distances between the microcrack and inclusion after rescaling. The scaling factors depend on the relative distance $s(|X_C - X_I|)$ according to a power law with exponent -2.

4 CONCLUSIONS

The total stress and strain fields show to be non additive and the appropriate DOL's for stress, $\sigma_{nl}^{CI}(x)$ and for strain $\varepsilon_{nl}^{CI}(x)$, have been computed. Though in principle DOL's could have a complicated dependence on the relative distance between the microcrack and the inclusion, we found that they obey a simple scaling law. We therefore propose the following model for the total stress field of a interacting pair consisting in a microcrack and in a hard inclusion:

$$\sigma_{zz}^{CI}(x) = \sigma_{zz}^{C}(x) + \sigma_{zz}^{I}(x) + (X_C - X_I)^{-2} \cdot [g_C(X - X_C) + g_I(X - X_I)] \quad (3)$$

where $g_C(X-X_C)$ and $g_I(X-X_I)$ are two suitable functions localized at the microcrack and at the inclusion, respectively. Similar expression is valid for strain components, as well.

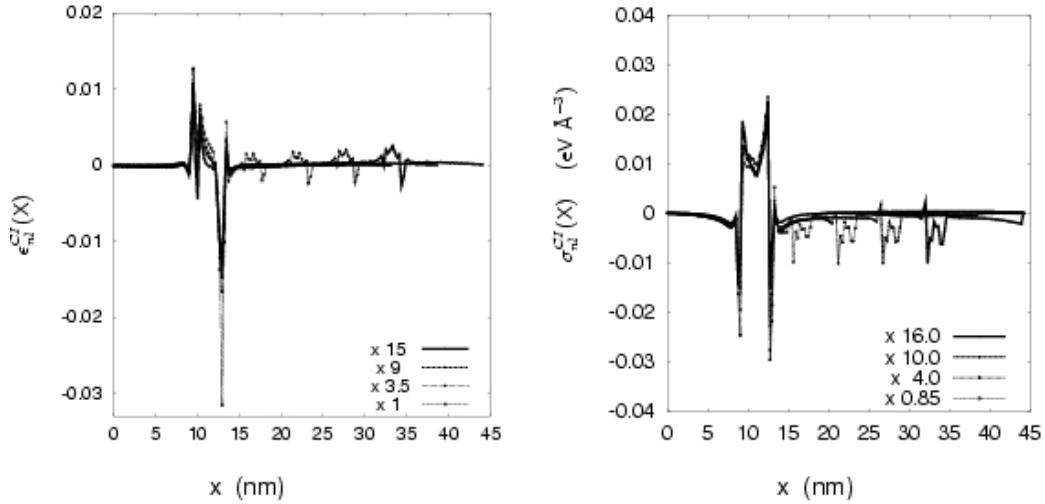

Figure 5: $\varepsilon_{nl}^{CI}(x)$ (left panel) and $\sigma_{nl}^{CI}(x)$ (right panel) profiles corresponding to four relative distances between the microcrack and the inclusion (see text).

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