MOLECULAR DYNAMICS STUDIES OF BRITTLE FRACTURE OF SiO$_2$

Q. H. Tang* and L. P. Cui

ABSTRACT

By applying for molecular dynamics (MD) simulation and Griffith fracture criterion, the brittle behavior of crack extension of mode I type is investigated. The critical stress intensity factor (SIF) K_{Ic}^{MD} of crack extension is calculated, and the evolution of atoms near crack tip is observed. It is found that K_{Ic}^{MD} is in good agreement with the Griffith fracture criterion $K_{Ic}^{Griffith}$.

Key Words: molecular dynamics; SiO$_2$; Griffith fracture criterion; brittle fracture

INTRODUCTION *(first-order heading)*

Brittle behavior of materials is a problem of longstanding interest for researchers. Sudden and rapid propagation of crack at nanometer and sub-micron level is attributed to the influence of a local stress field near the crack tip. The theory on brittle fracture was proposed by Griffith [1], and improved by Irwin [2] based on continuum mechanics. This theory could accurately predict the initiation of fracture, but can not account for atomic dynamics in the high-stress regions. It may be the proper way by employing MD to trace atomic behavior at the zone of crack extension. MD investigations of the fracture process in brittle materials have been carried out extensively. Swadene and Baskes [3] successfully performed the simulation of the brittle fracture in silicon and determined the way in which potential energy (strain energy) was converted into other forms. Many investigations on the fracture processes of α-SiO$_2$ have been carried out. Swiler and co-workers [4] pointed out that at the low strain rates, strain added uniformly to the structure is allowed to flow from higher density regions to lower ones. By using the classical 2-body potentials with considering the effect of charge-transfer, Muralidharan et al. [5] carried out MD simulation to study the fracture process of a prototypical brittle material, the growth of 'critical' voids was observed.

In this paper, MD simulation with TTAM potential is performed to investigate the brittle fracture of mode I type. It was found that the critical SIF obtained by MD simulation is consistent with that of the fracture theory analysis.

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COMPUTATION AND MODELLING

It is known that the accuracy of MD simulations is dictated by the accuracy of the interatomic potentials being used. Watanabe et al. [6] proposed an interatomic potential for Si/O mixed system which was an extension of the Stillinger-Weber (SW) potential of silicon. The modified SW potential has three-atom contributions and the computation process is very complex. TTAM [7] potential function is the pair potential and is widely accepted. Considering the computational efficiency, TTAM potential is used to describe interatomic interaction in this article.

The modulus of silica is determined by the uniaxial extension of MD simulation. Both the strain and the stress are calculated. The stress is computed according to the formula given by Alber et al. [8]. The curve of stress versus strain is plotted in Fig.1. Based on our calculation and isotropic continuum analysis, the elastic modulus $E= \sigma_{zz}/\varepsilon_{zz}$=300 GPa, and Poisson ratio v is nearly zero which is similar to that of Kimizuka and Kaburaki [9]. The shear modulus G=150 GPa.

The parallelepiped with a slit is used as the simulation model of the crack and the sizes of x, y, and z directions are 233.6, 7.3 and 116.8 Angstrom, respectively. The length of the crack is 60 Angstrom and the width 6 Angstrom. The schematic diagrams are shown in Fig.2a. The periodic boundary condition is adopted in y direction and the fixed displacement boundary condition is in x, z directions [10]. The displacements of atoms in boundary region are dictated by mode I type with K_I field in x-z plane [12]. The time integration of motion is performed by Verlet algorithm, and the time step Δt=1.0 fs. The MD simulation is with the temperature of 300 K.

RESULTS AND DISCUSSION

The evolution of atom configurations near crack tip is plotted in Fig.2. When t=0 ps, the atoms are in the initial state; when t = 90 ps, crack length increased a little and crack opening is from 6 Angstrom increased up to about 21 Angstrom. Near the crack tip atoms were in the state of disorder and the micro-voids were nucleated. The failure of simulation material β-SiO$_2$ accelerates crack extension. At this time stress is up to 13.4 GPa which is in the critical state of crack extension; and the strain energy stored in the simulation system is up to the maximum and is ready to release out for crack extension. As the applied loading increased continuously, the crack begins to propagate. In the front of crack tip a lot of voids forming, growth and coalescence due to the higher stress and strain. When t=300 ps, the crack opening increases up to 50 Angstrom and the crack length is about 15 Angstrom. Fig.2c displays crack extension by the void-void coalescence and connection of voids and crack. The results are similar to those of SiO$_2$ MD simulations by Muralidharan et al. [5]. The curve of stress versus the SIF is plotted in Fig.3. When the SIF is about 1.8 MPam$^{1/2}$, the stress dropped suddenly and the SIF at this time is defined as the critical value of crack extension K_{Ic}^{MD}. It is about t = 90 ps and the evolution of atom configuration is plotted in Fig.2b. Based on the continuum mechanics Griffith proposed the critical condition of crack extension $K_{Ic}^{Griffith}$ by

CONCLUSION

MD simulation is carried out in order to understand the behavior of crack extension of a brittle material β-SiO_2. Thecrack extension is observed due to the void-void coalescence and connection of voids and crack. The critical SIF calculated by MD is in good agreement with that of Griffith fracture analysis.

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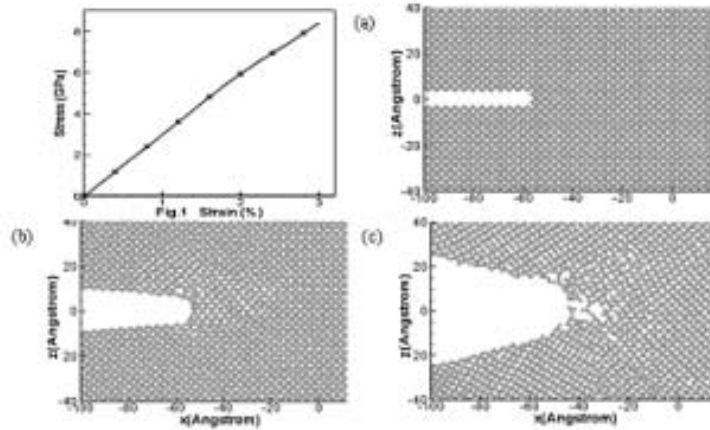
Fig.1 Curve of Stress versus Strain; Figure 2. Configuration
evolutions of the atom near

which crack extension could be predicted [1].

$$K_{Ic}^{Griffith} = 2\sqrt{G\gamma_s/(1-\upsilon)} \quad (1)$$

where $K_{Ic}^{Griffith}$ is the critical SIF, γ_s is the surface energy, and both the shear modulus G and Poisson radiov were obtained brfore. The surface energy of SiO_2 is computed in such a way. The sample containing 12288 atoms is selected and the size of x, y, and z axes are 58.4, 58.4, and 58.4 Angstrom, respectively. First, the total potential energy ϕ_1 of system was calculated with periodic boundary condition along x, y and z directions as system is in the equilibration state; then the total potential energy ϕ_2 of system was calculated with non-periodic boundary condition along z direction. The surface energy is obtained $\gamma_s = (\phi_2 - \phi_1)/2S_{xy}$, where S_{xy} is the area of plane xy. The surface energy is calculated, γ_s=5.119 J/m². Substituting the shear modulus, Poisson radio and surface energy into equation (1), the critical SIF is $K_{Ic}^{Griffith}$=1.75 MPam$^{1/2}$. According to Griffith criterion of crack extension, when the SIF is up to $K_{Ic}^{Griffith}$, the crack begins to propagate. The result of Griffith theory is in good agreement with that of our MD simulation K_{Ic}^{MD}=1.8 MPam$^{1/2}$.
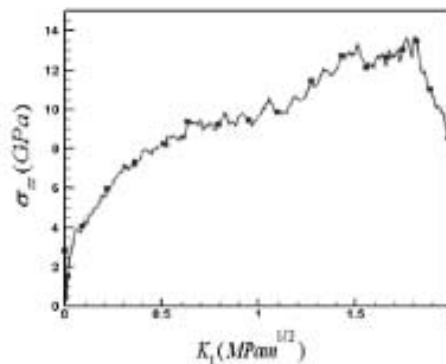

Figure 3. Curve of stress versus stress intensity factor