Computational Materials Science 124 (2016) 151–159

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

The spallation of single crystal SiC: The effects of shock pulse duration

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ARTICLE INFO

Article history:
Received 13 May 2016
Received in revised form 22 July 2016
Accepted 24 July 2016
Available online 5 August 2016

Keywords:
Shock
Spallation
Plasticity
Duration

ABSTRACT

Shock-induced spall in initial defect-free single crystal SiC is investigated using molecular dynamics (MD) simulation. Three shock pulses ranging from triangle to square are adopted to study the effects of pulse duration on spallation. The evolution of micro-structure and damage are analyzed in detail. Shock-induced plasticity is found to include deformation twinning and structure changes from 4 to 5 fold coordination number. These deformations disappear upon unloading causing numerous defects. Morphology of spallation is found to depend on these damage strongly. Furthermore, the spall strength obtained from free surface velocity and bulk are compared. Triangle pulse yields a higher value in the spall strength calculated from free surface velocity, while square pulse enjoys a similar result in both methods. Moreover, the theoretical total spall thicknesses are derived basing on the theory of spallation. The prediction of the total spall thicknesses are made using the stress waveform right before reflection and the spall strength. A good agreement between the simulation and the prediction is found in triangle wave.

1. Introduction

High performance ceramics (AlN, SiC, and Al_2O_3) are regarded as promising engineering materials because of their excellent chemical and physical properties including high strength, high hardness and high stiffness. They are widely used in shock protection system, such as the coating of armor [1,2] and the aerospace facilities like spacecraft and space station which are at risk of being super-high speed impacted by the micrometeorite [3–5].

In view of its utilization in extremely harsh environment, several studies have been carried out to investigate the mechanical behavior of these ceramics under high speed impact. Such events accompany with very high shock velocity and high strain rate which make it difficult or at least high cost to have such experiments, although nowadays researchers can achieve velocity above 16 km/s using a two-stage gas gun [6] and produce high strain rate ($\sim 10^7\ s^{-1}$) via laser driven impact [7,8]. On the other hand, both macro-and micro-structural characteristics are known to act as an essential role in defining a shock response of material. It is very important to understand the microscopic process including deformation, damage and fracture behaviors in ceramics. Molecular dynamic (MD) simulation provides a means to realize analysis at atomic level. Atomic mechanisms of fracture accompanying structural phase transformation in AlN ceramic under hypervelocity impact have been investigated using large scale MD simulation [9,10]. The interaction between the reflected elastic wave and the structural phase transformation wave has been found to lead to nano-voids and dislocation which relate to cracks. Planer shocks have also been applied to AlN to study the nanoscale structure of shock waves in high strength ceramics [11]. Shock Hugoniot curves have been calculated along different crystallographic directions which illustrate three shock response regimes. Hypervelocity impact has also been applied to Al_2O_3 ceramics to investigate the deformation mechanisms using MD simulations [12–14]. A wide range of deformations including slip and twins have been found to emerge and disappear as a function of time under the influence of local stress fields. Subsequently, defect free sapphire and sapphire with micro-crack have been considered to investigate the formation of twins under shock wave loading by Kuksin and Yanikin [15]. As to the SiC ceramics, a series of hypersonic velocity impacts on a-SiC target and CNT/a-SiC have been done to investigate the penetration depth as a function of impact velocities [16–18]. Nanoductility induced brittle fracture in 3C-SiC ceramics under hypervelocity projectile impact have been carried out in a large MD simulation [19]. The shock-induced structural transformation to plastic deformation and brittle fracture have been described. Recently, plane shocks loading on 3C-SiC [20,21] have been done, which reveal the interplay between elastic compression, plastic deformation and the structural phase transformation. Although these studies have shown much information about the high performance ceramics, they mostly focus on shock

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http://dx.doi.org/10.1016/j.commatsci.2016.07.028
0927-0256/

compression process, while the tensile fracture evolution resulting from the interaction between the reflected wave and unloading wave still lack information. Spall fracture is a shock-induced dynamics fracture phenomenon, which is of practical importance in virtually all applications involving rapid loading by explosives, impact. Besides, there are many factors that influence the spall damage, involving not only shock intensity and micro-structure, but also loading rates and shock wave profile. It is also of scientific importance in studies of elementary strength of materials because the extremely high loading rates make it possible to attain stress levels that approach the theoretical strength of the material [22] and give information in the effects of strain rate on it.

In this work, the effects of shock pulse on spallation are investigated using MD simulation as a complement to the research of materials under high shock intensity and extremely high strain rate loading. We focus on the evolution of micro-structure during the compression and tensile process under different shock durations. The micro-plasticity and the micro-cracking are analyzed. The spall strength calculated from the free surface velocity indirectly and that obtained from the bulk sample directly are compared and discussed. The spall thickness is predicted using spall theory and compared with simulation results. The outline of this paper is as follow. Section 1 mainly presents overview of high velocity impacts on high performance ceramics using MD simulations. Section 2 covers the details of simulation and the spall thickness derived from spall theory. In Section 3, simulation results are presented and discussed in detail. Finally, the conclusions are given in Section 4.

2. Method and theory

2.1. Simulation setup

The MD simulations are carried out to investigate the shock-induced spall in single crystal SiC. An effective interaction potential proposed by Vashishta [23] is employed in our simulations. The potential takes into account the ionic and covalent nature of bonds by including screened Coulomb, charge-dipole, Van der Waals interactions, steric repulsion, and three-particle potential for bond bending and stretching. The potential is successfully applied in high pressure and high temperature conditions [9–14]. Since the Vashishta potential is not yet available directly in MD code LAMMPS (Large-Scale Atomic/Molecular Massively Parallel Simulator) [24]. The additional potential files should be developed to make it possible to run the MD simulation in LAMMPS as what Kuksin and Yanikin [15] have done in their researches. The potential consists of two-body and three-body terms.

$$E = \sum_{i<j} V_{ij}^{(2)}(r_{ij}) + \sum_{ij<j} V_{jik}^{(3)}(r_{ij}, r_{ik}, \cos\theta_{jik}) \tag{1}$$

where E is the total potential energy of the system, $V_{ij}^{(2)}(r_{ij})$ is the two-body term, $V_{jik}^{(3)}(r_{ij}, r_{ik}, \cos\theta_{jik})$ is the three-body term. $r_{ij} = |\vec{r}_{ij}|$, $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$. $\cos\theta_{jik} = \vec{r}_{ij} \cdot \vec{r}_{ik}/r_{ij}r_{ik}$, and r_i is the position of the atom i. The two-body term is given by

$$V_{ij}^{(2)}(r) = \frac{Hij}{r^{\eta ij}} + k_e \frac{Z_i Z_j}{r} e^{-r/\lambda} - k_e \frac{Dij}{2r^4} e^{-r/\xi} - \frac{W_{ij}}{r^6} \tag{2}$$

where Hij is the strength of the steric repulsion, Z_i is the effective charge, Dij is the strength if the charge-dipole attraction, W_{ij} is the van der Waals interaction strength, η_{ij} is the exponents of the steric repulsion term, k_e is the Coulomb constant. λ and ξ are the screening lengths for Coulomb and charge-dipole terms, respectively. The three-body term is given by

$$V_{jik}^{(3)}(r_{ij}, r_{ik}, \cos\theta_{jik}) = R^{(3)}r_{ij}, r_{ik}P^{(3)}\theta_{jik} \tag{3}$$

where

$$R^{(3)}r_{ij}, r_{ik} = B_{jik} \exp\left(\frac{\gamma}{r_{ij} - r_0} + \frac{\gamma}{r_{ik} - r_0}\right)\Theta(r_0 - r_{ij})\Theta(r_0 - r_{ik}) \tag{4}$$

$$P^{(3)}\theta_{jik} = \frac{\left(\cos\theta_{jik} - \cos\overline{\theta}_{jik}\right)^2}{1 + C_{jik}\left(\cos\theta_{jik} - \cos\overline{\theta}_{jik}\right)^2} \tag{5}$$

where B_{jik} is the strength of the interaction, $\Theta(r_0 - r_{ij})$ is the step function. γ, r_0, C_{jik} and $\overline{\theta}_{jik}$ are constants. All the parameters are adopted from Ref. [23].

The simulation domain containing about two million atoms is about $\sim 12\,\text{nm} * 12\,\text{nm} * 130\,\text{nm}$ along the x-, y-, and z-directions, respectively. The corresponding crystal directions are [1 0 0], [0 1 0] and [0 0 1] along the x-, y-, and z-directions. In order to eliminate the edge effects on the shock waves, periodic boundary conditions in x and y directions and free surfaces along the z direction are adopted. Plane shocks are used to control the shock compression and the long dimension of system, along the z direction is the shock direction. Thus, the model corresponds to a one-dimensional strain shock loading problem.

Before shock loading, the simulated system is relaxed at 300 K for 10 ps in the NPT ensemble to reach an equilibrium state to ensure that the residual stresses in the relaxed system are negligible when they are compared to the shock intensities. Then, a shock wave is generated by moving a piston at the left side toward the sample in NVE ensemble. The similar methods are adopted in other spallation simulations [25]. In order to investigate the effects of shock pulse on spallation, three shock durations (5.0 ps, 7.5 ps and 10.0 ps, respectively) are adopted in our work which finally generate different waveforms from triangle to square. After the piston is removed which means an unloading process, the loading surface becomes a free surface which is the same as the right side of the sample. Then a shock pulse propagating in the target is generated. As the shock pulse reaches the free surface, a reflected rarefaction wave is generated. The interaction of the reflected rarefaction wave and the unloading rarefaction wave results in tensile stresses. The fracture occurs when the tensile stress exceeds the spallation strength.

The binning analysis along the shock direction is adopted. The width of each bin is twice the lattice constant. The average physical quantities including stress, particle velocity, density profiles along the shock direction are obtained by averaging over the atoms in each bin. The local deformation and the structure changes are characterized by means of coordination analysis. The coordination number (CN) of atoms is calculated based on a given cut-off radius of 2.1 Å.

2.2. The spall thickness derived from theory of spallation

For a square wave with l width, the time that the wave just reaches the free surface is set to be t = 0. Subsequently, the compression wave front is reflected into tensile wave. The compression wave and the tensile wave that share the same amplitudes encounter with each other resulting in a region with zero stress until $t = \frac{l}{2 \cdot C}$. Where C is the wave speed. After that, the tensile region occurs. The spall begins when it meets the following conditions:

$$|\sigma_m| \geqslant |\sigma_s| \tag{6}$$

where σ_m and σ_s are the peak stress and the spall strength, respectively.

And the spall thickness (δ) can be easily calculated: