Acta Materialia 140 (2017) 274–289

Contents lists available at ScienceDirect

Acta Materialia

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

Full length article

Shock-induced spall in single and nanocrystalline SiC

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ARTICLE INFO

Article history:
Received 2 May 2017
Received in revised form
17 August 2017
Accepted 18 August 2017
Available online 25 August 2017

Keywords:
Silicon carbide
Spall
Shock wave
Structure phase transformation
Plasticity

ABSTRACT

Shock-induced spall in SiC is investigated via high strain-rate loading molecular dynamics simulations. The dynamic response under different shock intensities is characterized along the low-index 3C-SiC crystallographic directions, [001], [110], and [111], and in a nanocrystalline sample with 5 nm average grain size. The simulation results show that all single crystal samples generate elastic, plastic, and structural phase transformation waves for increasing particle velocities in good agreement with previous investigations. However, crystal anisotropy effects affect the exact shock response and the corresponding wave structures. The Hugoniot elastic limit is significantly higher along the [111] and [110] directions while the patterns of plastic deformation, based on deformation twinning, contrast along the three crystallographic directions. The spall behavior, both for single and nanocrystalline samples vary from classical to micro-spall. The predicted spall strength is at maximum along the [111] direction, at 34 GPa, followed by the [110], and [001] directions, at 32 and 30 GPa, respectively. Nanocrystalline SiC displays a spall strength over 66.7% lower than single crystals. Spall strengths from direct and indirect methods agree well for both classical and micro-spall regimes after applying an elastic-plastic correction and considering the change in sound velocity, in particular for the case where the structural phase transformation occurs.

1. Introduction

Silicon Carbide (SiC) has outstanding physical properties, such as low density, high stiffness, high hardness and high thermal conductivity, which makes it a desirable versatile engineering material. It is widely used in wear resistant [1], electronic [2], and shock protection applications [3,4], in particular in aerospace applications where it is used for protection against hypervelocity impact of micrometeorites [5–7].

An important phenomenon related to the shock protection applications of SiC is shock induced spall. Spall is a complex phenomenon involving dynamic fracture, disintegration, and ejection of fragments resulting from shock-induced damage following the propagation and release of strong shock waves. Spall has a crucial role in the application of many materials, structures, and designs such as armor coating, which are subjected to intense shock loading. A deep understanding of spall is critical for the design, construction, and use of systems which will be subjected to extremely high strain-rates. It is also of high importance in virtually all applications involving the use of explosives and high velocity impacts. According to whether a solid-liquid phase transformation occurs for metals before cavitation starts, spall phenomenon can be divide into two main categories, classical spall and micro-spall [8]. Micro-spall occurs when the shock loading is strong enough to melt the material. When that occurs regular oscillations of the surface velocity of the solid material are absent and only an approximatively constant value of spall velocity is observed as a function of time. Furthermore, micro-spall is usually accompanied by a significant amount of micro-scale ejecta. In contrast, in the classical spall regime the surface velocity displays regular oscillations due to reflections at the free surface and only a limited number of spall failure surfaces occur.

Fundamental shock loading experimental studies on SiC have been performed providing essential understanding of the shock compression and the Hugoniot Elastic Limit (HEL) of SiC [9–13] as well as the penetration response as a function of impact velocity [14]. In one of the experiments, an intriguing anomalous increase of the SiC strength above the HEL was reported [13]. Spall tests [15–20] reported a consistent trend of initial increase in the spall

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http://dx.doi.org/10.1016/j.actamat.2017.08.036
1359-6454/

strength followed by a decline with increasing shock pressure. In experiments with SiC sintered by spark plasma sintering (SPS) [20], the reported spall strength reportedly increased from 1.4 GPa to 1.5 GPa at low compressive stress, while at higher shock stress at 21.5 GPa, it degraded monotonously towards ~ 0.34 GPa. Besides, the spall strength of the sintered materials reported elsewhere [16] was systematically lower than that of SPS-processed SiC, arguably because of the coarse structure of the sintered SiC [20]. The spall strength of these SiC ceramics was found to increase from 0.9 to 1.3 GPa as the shock stress increased to 3.8 GPa. The increase of the impact stress above 5.8 GPa was accompanied by the decline of the SiC spall strength. As to the hot pressed SiC [15], below peak stress of about 7 GPa, its spall strength values are roughly twice lower than those of SPS-processed SiC. At higher peak stresses, however, the spall strength of the two materials become comparable. Other investigations reported values of the SiC spall strength even lower [21] indicating a strong influence of the manufacturing technique, and the density of defects and impurities, on the dynamic strength. A recent study on reaction-sintered SiC under planar impacts showed that spall strength of highly rigid ceramics varies non-monotonically with increasing compression stresses in the range 3–19 GPa [22]. Interesting, the performances of the ceramics were found to be very sensitive to the strain-rate loading [26], as well as transverse stress [27]. In view of its utilization in extremely harsh environment and shock protection, more studies of SiC under very high strain-rates are desirable to further clarify the deformation, damage and fracture phenomena. That is particularly relevant since current shock loading technology can achieve impact velocities above 16 km/s using two-stage gas guns [23] and produce strain-rate as high as 10^7 s^{-1} by laser driven shock loading [24,25].

While experiments are essential in evaluating the performance of devices, fundamental shock studies can be suitably investigated by large-scale atomistic simulations using molecular dynamics (MD). MD simulations can be used to simulate accurately the propagation of very strong shocks generating ultrahigh strain-rates above 10^7 s^{-1}. Extremely high loading rates make it possible to attain stress levels that approach the theoretical strength of materials (the strength that the material would have in the absence of defects) [43]. MD simulations have been successfully applied to investigate shock loading damage in metals including Cu [28–31], Ni [32], Al [33,34], Pb [35,36], Tin [37], Fe [38–41], and Ta [42].

Large-scale MD simulations of shock loading have also been performed on some high-performance ceramics including AlN [44,45and46], Al_2O_3 [47–50], and SiC [51–56] to characterize the damage produced by hypervelocity impact of projectiles. Extremely high strain-rates and strong shocks by hypervelocity impact have been generated in these simulations corresponding to typical micro-meteoroid impact conditions found in space. These simulations highlight the essential role of the macro- and microstructure in defining the shock response of a material. The grain sizes were reported to influence the compressive yield strength [57], while the crystalline plasticity affect the performance of materials at high pressure and strain-rates [58]. MD simulations show its advantages in the detailed atomistic description of these phenomena. Not only they can directly reveal the atomistic scale damage mechanisms, but also, they are very convenient to directly obtain the local distribution and evolution of critical physical quantities such as stress, density and temperature. Atomic mechanisms of fracture and the nanoscale structure of shock waves in some high strength ceramics have been proposed in these simulations. However, they mostly focus on the shock compression processes, while atomistic details on the tensile fracture evolution resulting from the interaction between the rarefaction (reflected) wave and unloading wave is still largely unknown. The spall is a highly complex phenomenon that includes shock wave propagation, reflection at free surfaces, induced plasticity, micro-cracking, and fragmentation. Many factors influence the spall damage, including shock intensity and the microstructure, as well as the loading strain-rates and the shock wave profile [59].

The main purpose of this work is to study spall in defect-free single and nanocrystalline silicon carbide subjected to extremely high strain-rates produced by different shock intensities using non-equilibrium MD simulations. The focus is on the evolution of the spall with increasing shock stress and the related induced plasticity, nano-cracking, and phase transformations. The outline of this paper is as follow. Section 2 provides details of the simulations and the spall theory. In Section 3, simulation results are presented and discussed. Finally, the conclusions are presented in Section 4.

2. Methodology and theory

2.1. Simulation setup

All MD simulations are performed using the simulation package LAMMPS [60]. The interatomic forces are calculated using the effective force field developed by Vashishta et al. [61]. This force field includes screened Coulomb, charge-dipole, van der Waals, steric repulsion, and three-body interactions to describe accurately the bond bending and bond stretching of ionic and covalent bonds. The force field parameters were fit to reproduce an extended set of structural and dynamic properties of SiC [61]. In particular, it was fitted to reproduce the pressure induced structural phase transformation, which is essential for the shock loading simulations discussed in this work. This force field fitted to different materials was successfully applied in investigation of shock involving high pressure and high temperature conditions in AlN [44,45and46], Al_2O_3 [47–50] and SiC [51–56].

The simulations systems contain about 2.1 million atoms. The single crystal systems are created by replicating 30, 30, and 300 unit cells along the *x*-, *y*-, and *z*-directions. The crystal directions [001], [110] and [111] are aligned along the shock propagation *z*-direction, respectively. [100], [010] and [001] are aligned along *x*-, *y*-, and *z*-axis in the case of [001] shock direction; [00−1], [−110] and [110] are aligned along *x*-, *y*-, and *z*-axis in the case of [110] shock direction; and [2−1−1], [01−1] and [111] are aligned along *x*-, *y*-, and *z*-axis in the case of [111] shock direction. As to the nanocrystalline SiC, the long length of the sample is also aligned along the shock propagation *z*-direction. The nanocrystalline sample used in this work is generated by the Poisson-Voronoi method. A set of seeds are first distributed in the simulation supercell randomly as Voronoi centers ($3 \times 3 \times 26$ grains are located along *x*-, *y*- and *z*-directions, respectively). Associated with each seed is a rotation matrix. The Voronoi cells are generated using an open utility [62] and finally the nanocrystalline sample is generated. There are a total of 234 grains with an averaged 5 nm grain size in the nanocrystalline sample. To eliminate edge effects in the shock waves, periodic boundary conditions are applied along the *x* and *y* directions while free surfaces are imposed along the *z* direction. The shock compression is performed generating plane shock waves that propagate along the long dimension of the system aligned in the *z*-direction.

Before shock loading, the simulated systems are relaxed at 300 K for 10 ps in the NPT ensemble to reach an equilibrium state and ensure that residual stresses are negligible. Then, a shock wave is generated by moving a flat surface infinite mass piston against one of the free surfaces of the sample. From this point the simulation proceeds with a fixed MD box and no temperature control is applied. In this work, we generate shock pulses following typical shock experiments, to properly induce and investigate the spall process, i.e. the piston moves into the system for 7.5 ps generating a