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Shock loading on AlN ceramics: A large scale molecular dynamics study

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ABSTRACT

The nanoscale structure of shock waves in high strength AlN ceramics is studied using molecular-dynamics simulations. Impacts using four independent crystallographic directions, with particle velocities in the range 0.8–4.0 km/s, reveal the generation of a well-defined two-wave structure, consisting of an elastic precursor followed by a wurtzite-to-rocksalt structural transformation wave (STW). Impacts with particle velocities below 0.8 km/s or above 4.0 km/s generate single elastic or single overdriven shock waves, respectively. The latter propagates faster than the longitudinal sound velocity along the impact direction. The structure of the STW exhibits a strong anisotropy with respect to the crystallographic directions. Results show distinct shock front features from a steady, sharp and well defined STW front for impact at the basal plane to a rough STW front with the formation of an intermediate metastable fivefold coordinated phase or the generation and propagation of dislocations from the shock front for impact at other directions. These results indicate that shock-induced damage in brittle materials can be highly intricate even in defect-free systems. Simulations show no deformation twinning or other well defined plastic wave as found in experiments on polycrystalline AlN suggesting that interfaces and defects strongly affect the materials response to shock loading.

1. Introduction

Molecular-dynamics (MD) simulations of shock waves have been performed for over three decades to test the validity of shock wave theories and to provide microscopic details of shock propagation (Holian, 1988; Holian et al., 1980; Holian and Straub, 1979). Early simulations were performed in simple solids and liquids to investigate the nature of shock waves such as the shock evolution and shear stress relaxation mechanisms. Later, they were used to describe complex phenomena such as multi-shock wave structures induced by polymorphic phase transitions (Robertson et al., 1991), and intricate energetic materials supporting chemically sustained shock waves (Brenner et al., 1993).

Large scale MD simulations of shock wave present a new dimension for the description of shock phenomena, narrowing the gap between experimental studies and microscopic models of shock phenomena. Using large scale simulations, plastic deformations on the shock front in metallic systems can finally be described in fine details along with the rich dynamic nano-structures left behind the shock interface (Holian and Lomdahl, 1998). Details of the shock propagation in metals along multiple crystallographic directions (Bringa et al., 2004; Germann et al., 2000, 2004), as well as the shear stress released by nucleation of complex dislocation structures (Tanguy et al., 2003), and induced structural phase transitions (Kadau et al.,

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2002) can be described accurately. Large scale MD simulations were also employed successfully to describe the strength of nanocrystalline metals under shock (Bringa et al., 2005).

Recently, the interest in studying shock effects in high strength ceramics has increased because of potential application of these materials as coatings for improved light weight armor designs. The literature of experimental studies of these ceramics is extensive and includes shock experiments on a wide range of materials such as Al_2O_3, B_4C, SiC, Si_3N_4, and AlN (Dandekar, 1994; Dandekar et al., 1994; Gorelskii et al., 2000; Grady, 1994, 1998; Kanel et al., 2009; Kipp and Grady, 1994; Mashimo et al., 1999b; Rosenberg et al., 1991).

Due to intrinsic differences in physical and chemical properties there can be large differences between the shock behavior among different classes of solid materials, e.g. metals and ceramics. While the previously cited MD simulations of shock in metallic materials are instructive and provide a good framework to further investigations, MD simulations of shock in ceramics must be performed to describe the distinct features of shock loading in this class of materials. While MD simulations of projectile impact were previously employed to investigate the generation of damage and fracture in AlN ceramics (Branicio et al., 2006, 2008) there is still a lack in the understanding of the shock induced features in AlN and other ceramics. Shock loading experiments in AlN have shown the generation of a complex set of multiple wave structures including a plastic and a structural transformation wave (Mashimo et al., 1999b). However, it is not clear from a nanoscale and atomistic point of view, how a shock pulse is absorbed in AlN, how it generates different types of wave structures and how does that depend on the shock intensity. It is also not clear what are the effects of shock loading direction considering different crystallographic directions of a single AlN crystal and what are the effects of grain size and grain boundaries in the shock propagation and generation of plastic deformation.

In this work we aim to address some of these questions performing large MD simulations in a well defined and controlled shock loading environment using plane shocks in defect free single crystals of AlN. We employed a wide range of shock intensity from very weak shocks generating particle velocities $u_p \sim 100$ m/s, to very strong shocks with $u_p \sim 5$ km/s. The forces among atoms are calculated from a many-body interatomic potential validated by experimental results on lattice constants, elastic moduli, cohesive energy, and melting temperature (Vashishta et al., 2011). A more stringent validation of the potential is provided by the wurtzite-to-rocksalt structural phase transition in AlN. High-pressure experiments reveal that this transformation occurs at ~20 GPa (Mashimo et al., 1999a) which is close to the calculated value of 25 GPa. This potential has been used successfully to describe shock-induced damage and fracture in projectile impacts on AlN (Branicio et al., 2006, 2008). The same potential form has also been successfully applied to describe the mechanical behavior of similar ceramics such as SiC (Branicio, 2012; Branicio et al., 2010; Kikuchi et al., 2005; Rino et al., 2004; Tsuzuki et al., 2011) and Al_2O_3 (Zhang et al., 2007a,b, 2008).

2. Methods and simulation procedures

The simulated systems are AlN single crystal slabs of about $15 \times 15 \times 200\ nm^3$ dimensions containing 4 million atoms. The long system dimension, along the z direction, is aligned with the impact direction to allow the shock waves to develop for at least 15 ps. Before impact, the crystalline structure of the target material is a defect-free wurtzite. In order to perform impact on different crystallographic orientations of the wurtzite crystal, the slab is oriented in such a way that the z-axis, chosen as the impact direction, is parallel to one of the low index orthogonal crystallographic directions: $[0\,0\,0\,1]$, $[1\,1\,\bar{2}\,0]$, and $[1\,0\,\bar{1}\,0]$. An additional oblique direction, with an irrational Miller index, is prepared to access the shock response of the system out of the low-index crystalline directions. It is prepared from a system initially with directions x, y, and z aligned with $[1\,0\,\bar{1}\,0]$, $[1\,1\,\bar{2}\,0]$, and $[0\,0\,0\,1]$, respectively, rotating the crystal clockwise by 62° on the z–x plane. Therefore, the oblique impact direction is perpendicular to the $[1\,1\,\bar{2}\,0]$ direction and parallel to the $[0\,0\,0\,1]$–$[1\,0\,\bar{1}\,0]$ plane, making an angle of 62° with the $[0\,0\,0\,1]$ direction. To construct such an oblique system while keeping periodicity, and avoiding introducing new surfaces, a large 472-atom super cell is defined from within the rotated crystal in order to generate negligible residual stress. The calculated residual shear stress for the oblique supercell is less than 0.3 GPa and is orders of magnitude smaller than those generated during the shock simulations. All simulations are performed with periodic boundary conditions in the x and y directions and free surfaces along the z direction. The particle velocity, which here is the same as the impact velocity, is in the range of 0.2–5 km/s, and it accesses all shock wave regimes and induced shock pressures up to 150 GPa. The equations of motion are numerically integrated using the velocity-Verlet algorithm with a time step of 1.5 fs. For the range of impacts velocities investigated this time step is small enough to allow stable integration of the equations of motion for all atoms and the conservation of the energy during all simulations to at least the third meaningful digit. Simulations are performed with systems initially at $T = 10$ K and $T = 300$ K to evaluate the effect of temperature in the shock Hugoniot. After the systems are initially equilibrated shock simulations are performed in the NVE ensemble. The planar impact simulations are performed in the reversed geometry with the system target hitting the piston at a fixed position with a chosen impact velocity. The piston is a hard wall, which instantly bounces any particle hitting its surface by inverting the component of the momentum perpendicular to the hard wall. Shock profile of properties is calculated along the system in the impact z direction. Bins 5 Å wide are used to average local quantities and quantify the shock profile which here includes the particle velocity, stresses, internal energy, displacement in the xy plane, and density. Particular care is taken in the calculation of the latter. The usual method of direct average of atoms on bins is replaced by the average of the inverse atomic Voronoi polyhedral volumes. Such volumes calculated from the Voronoi tessellation (Brostow et al., 1978; Finney, 1979; Tanemura et al.,