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Surface damage of CuZr metallic glass by hypervelocity nano-projectile: A molecular dynamics study

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ABSTRACT

In this study, molecular dynamics simulation is employed to explore the surface damage of CuZr metallic glass under the impact of nanosized hypervelocity projectile. Collision of the projectile leads to formation of impact-craters, which modulate the surface morphology of the amorphous target. The computations provide a close view of the mechanism of cratering and allow a quantitative analysis of the damage features. In addition, the effect of damage on the mechanical behavior of the material is evaluated through simulated nanoindentation of the impact craters. The simulations reveal that both morphological and mechanical properties of the metallic glass surface depend upon the impact velocity of the nano-projectile.

1. Introduction

High-speed impact of nanosized clusters and particles on solid surfaces has drawn wide interest in recent years. Such studies are often motivated by their relevance in several applications, like bombardment of micrometeorites [1,2], armor design [3,4], surface modification [5,6], and ballistics [7,8]. In particular, the progress in cluster beam technology [9] has also necessitated a deep understanding of the damage and behavior of a solid surface under the impact of small atomic clusters. As the experimental studies are known to offer only a limited scope of information in this regard, several studies have resorted to atomistic simulations to gain an insight into the dynamics of these collision processes. Capabilities of such simulations in capturing the atomistic scales of length and time are particularly fruitful in revealing the transient parts of such ultrafast processes. Owing to this advantage, the molecular dynamics (MD) simulations have been carried out to mimic the bombardment of nanoclusters on several types of materials. At one hand, they are known to exhibit the formation of crystal-defects in ceramics [10], while at the other, they yield the penetration-depths of projectile atoms in amorphous targets [11]. Moreover, the techniques of computer simulations have also been employed to study the brittle fracture in silica glasses [12,13]. Recently, molecular dynamics computation employing the reactive force field model has succeeded in unveiling the mechanochemical properties of graphene under the bombardment of nano-projectile [14].

Apart from ceramics and glasses, understanding the effects of nanocluster bombardment on metallic solids is extremely significant on account of their widespread technological applications. This has led to extensive simulations of impact of nano-projectiles on metallic targets. In terms of their motivations, we can broadly categorize the relevant studies into two groups. In the first, the simulations are done with the aim of understanding the phenomenon of cluster deposition. For instance, Alamanova et al. [15] and Zhang et al. [16] have simulated the deposition of copper nanoclusters on copper and iron substrates, respectively. More recently, molecular dynamics (MD) simulations of collisions of Cu-nanoparticles with aluminum target have been carried out [17]. The simulations demonstrated that even for much larger nanoparticles, good adhesion was possible at elevated temperature, provided that the impact velocity was moderate. In the second group of studies, the simulations are primarily aimed at investigating the severity of surface damage caused by energetic nanoparticles. An example is the work by Amigo et al. [18], which focused on the structural changes and temperature variations undergone by a copper target, when hit by a high-velocity Cu nano-projectile. In comparison to the simulations by Pogorelko et al. [17], Amigo et al. [18] employed a much smaller nanoparticle as the projectile. Nevertheless, as their study covered the hypervelocity regime, the per-atom energy was larger by two orders of magnitude. Similarly, the work of Samela and Nordlund [19] attempted to bridge the gap between experimental observations

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and classical theory of sputtering of metals. They also succeeded in demonstrating the transition from atomistic to macroscopic mechanism of crater formation in metals [20].

In the context of previous studies, we can clearly notice a gap between the simulations of non-metallic and metallic materials. For example, Refs. [10] and [11] indicate that for ceramic materials, surface damage of both crystalline and amorphous targets have been simulated. However, for purely metallic systems, all the studies have hitherto dealt with crystalline metals only, while the effects of nano-projectile collisions with disordered metallic phases have remained unexplored. In some of the simulations [17,21], it has been demonstrated that a nanosized particle colliding with a metallic crystal leads to plastic deformation through the formation and movement of line defects. It is well known that unlike their crystalline counterparts which usually deform through dislocation-mediated slips of atomic planes, amorphous alloys can exhibit ductile failure through the formation of shear bands [22,23]. Therefore, it is expected that the surface damage of an amorphous metal caused by a nano-projectile would occur through an entirely different physical mechanism. In the present study, this aspect has been explored by means of MD simulations. A Cu-nanoparticle serves as the projectile, whereas the target consists of CuZr metallic glass. As the aim is to investigate the damage on the metallic glass surface, the hypervelocity regime has been selected for the projectile so that reasonably large impact-craters can be obtained. Apart from revealing the modality of surface damage at atomistic scales of length and time, the computations allow us to observe and quantify the morphology of the impact-craters. In addition, simulated nanoindentation has been carried out at the site of impact in order to assess the effect on mechanical behavior of the damaged surface.

2. Simulation scheme

All the simulations described here have been performed by using a Finnis-Sinclair type potential [24], which is specifically optimized for the CuZr metallic glasses. This EAM potential was originally created by fitting to experimental diffraction data and was found to reproduce the values of cohesive energies and formation enthalpies with satisfactory accuracy. Subsequent studies indicated that the elastic constants of metallic glasses obtained from this interatomic potential are reasonably close to the experimental values [25–27]. As a result, many of the recent studies [28–30] have employed this potential to investigate the elasto-plastic deformation of Cu-Zr metallic glasses. In this study, the metallic glass is created through the typical melt-and-quench technique [31]. A mixture of 479,992 atoms of copper and zirconium in the stoichiometric ratio of 1:1 is melted at 1800 K for 200 ps. The melt is then quenched to 50 K at a rate of 0.2 K/ps and the CuZr metallic glass is obtained. The target has final dimensions of 16.6 nm × 16.6 nm × 31 nm as displayed in Fig. 1. The projectile is in the form of a 1.6 nm diameter Cu-nanocluster consisting of 188 atoms and is placed at a height of several Angstroms above the top surface of the target. For the purpose of impact simulation, the target is partitioned into four layers along the z-direction (Fig. 1). Brief descriptions of all partitions are given below.

Fixed layer - The thin layer at the bottom consists of fixed atoms, whose positions are not allowed to vary with time. This rigid layer is necessary to prevent the vertical translation of the whole target due to impact of the nanocluster. It is the thinnest partition with a thickness of 0.5 nm.

Damping layer – This 4 nm thick layer is above and adjacent to the fixed layer. Beside the usual interatomic force, each atom in this layer experiences an addition force, $\mathbf{F} = -\gamma \boldsymbol{v}$, where $\boldsymbol{v}$ is the atomic velocity and $\gamma = 0.25$ eV·ps/Å^2 is a drag constant. As this force is always directed against the velocity of the atom, it has a damping effect which drains out the kinetic energy from the layer. The purpose of this layer is to attenuate the strength of pressure waves generated at the site of impact.

Isothermal layer – The 2 nm thick layer above the damping layer is maintained at a constant temperature of 50 K by means of velocity rescaling. It acts as a thermostat for the rest of the system and absorbs the excess heat generated as a result of bombardment of the metallic glass target by the high-velocity nanocluster.

Newtonian layer – Rest of the target above the isothermal layer is the active region. Unlike the other three layers, the atoms here simply follow the Newtonian dynamics without any additional artificial effect. The reason for separating the thermostat layer from this region is that the isothermal atoms tend to thermally equilibrate the system. However, a vigorous event like hypervelocity impact drives the system far away from equilibrium. Thus, separating the active region from the isothermal layer prevents the thermostat from directly interfering with the event, thereby mimicking a more realistic physical scenario.

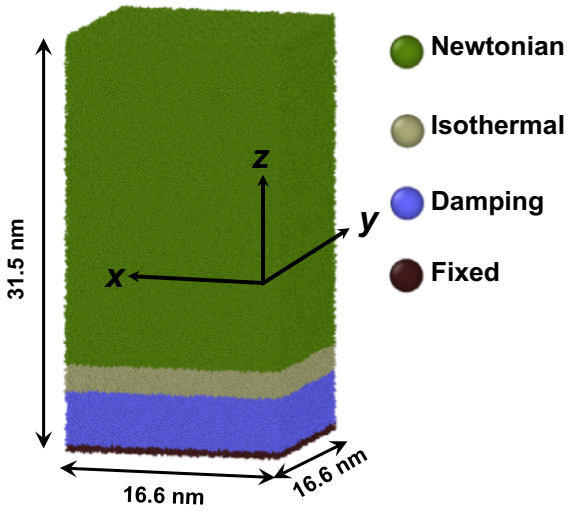

Fig. 1. Simulated metallic glass target with atoms colored according to the layers they belong to. Refer to the text for detailed descriptions of the four layers. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Once the system is set up, it is thermalized for 50 ps and subsequently, a downward velocity is imparted to the nano-projectile. The simulations are performed at velocities of 6–10 km/s. In this regime, the projectile's kinetic energy varies from 12 to 33 eV/atom, which is much lager than those in the deposition studies [15–17] and is rather comparable to those in Ref. [18]. Each collision simulation proceeds for 150 ps. As the process of crater formation is complete in the first few picoseconds, the total duration of 150 ps ensures a properly equilibrated system at the end of the simulation.

Mechanical behavior of the damaged surface is probed using a simulated nanoindenter. The same scheme of partitioning as shown in Fig. 1 is used here as well. The virtual indenter is spherical in shape and has a diameter of 60 Å. An atom within the spherical domain of the indenter experiences a radially outward repulsive force of magnitude $k(r - R)^2$, where r is the distance of the atom from the center of indenter, R is its radius and $k = 20$ eV/Å^3 is a force constant. The indenter is placed on top of the impact-crater and pressed against the target in the downward direction. The indenter is lowered at a constant rate of 5 m/s for