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Nucleation and Evolution of Dynamic Damage at Cu/Pb Interfaces Using Molecular Dynamics

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Abstract. *For ductile metals, the process of dynamic fracture occurs through nucleation, growth and coalescence of voids. For high purity single-phase metals, it has been observed by numerous investigators that voids tend to heterogeneously nucleate at grain boundaries and all grain boundaries are not equally susceptible to void nucleation. However, for materials of engineering significance, especially those with second phase particles, it is less clear if the type of bi-metal interface between the two phases will affect void nucleation and growth. To approach this problem in a systematic manner two bi-metal interfaces between Cu and Pb have been investigated: {111} and {100}. Qualitative and quantitative analysis of the collected data from molecular dynamics shock and spall simulations suggests that Pb becomes disordered during shock compression and is the preferred location for void nucleation under tension. Despite the interfaces being aligned with the spall plane (by design), they are not the preferred location for void nucleation irrespective of interface type.*

INTRODUCTION

Multi-phase alloys are one class of materials that are widely utilized in modern engineering applications. Some of these applications involve subjecting these materials to impact and dynamic loading. In the past, extensive research has focused on understanding the dynamic fracture response of both metals and alloys, especially in cases where the second phase additions are stiffer than the primary metallic phase. In case of these single-phase ductile materials, it is widely accepted that microstructure affects the response of a material to dynamic loading, since voids tend to nucleate at heterogeneities in the microstructure such as vacancies, cracks, inclusions, and grain boundaries [1, 2, 3, 4, 5, 6, 7]. However, less is understood about this effect under conditions of two-phase boundaries or at bimetallic interfaces.

Work by Minich et al. [5] on two phase materials like single crystal copper with SiO_2 inclusions shows that the presence of small, hard SiO_2 precipitates lowers the stress required to nucleate voids in this material as compared to that for pure Cu. Similarly, work by Christy et al. [8] that studies inclusions present at a grain boundary in Cu, reveal that voids prefer to nucleate at these inclusions along the grain boundaries. Hixson et al. [9] show an interface dependence of this phenomena based on the response of aluminum with alumina inclusions and within a Cu/Nb material. The spall strength of the Al/Al_2O_3 system is found to be lower than that of pure aluminum and is highly dependent on the volume fraction of inclusions and their specific particle morphology. On the other hand, the spall strength of a Cu/Nb system remains unchanged by the presence of 15 vol % Nb particles embedded in the Cu matrix in comparison to high purity copper. Recent spall experiments by the authors have also shown that addition of 1wt% Pb to Cu can decrease its spall strength by 50% [10]. Although these and other experimental observations show that the presence of a second phase can impact the spall strength of a material, the specific role of the bi-metal interfaces in damage nucleation and its evolution remain poorly understood.

To better understand the role of bi-metal interfaces on damage nucleation and evolution Molecular dynamics (MD) simulations have also been previously employed . However, at the atomistic scale of MD this problem must be cast in terms of a bi-metal interface or nano-precipitates at a grain boundary or within the material matrix. To the best of our knowledge only one MD study has focused on studying damage nucleation and evolution at a bimetal interface under shock loading conditions. This study focused on two types of interfaces in Cu/Nb: $\{112\}_{Cu}/\{112\}_{Nb}$ and $\{111\}_{Cu}/\{110\}_{Nb}$. In the former interface, the threshold for nucleating Shockley partials in Cu was found to be lower than that to transmit partials from Cu to Nb, whereas the barriers for these two events were found to be comparable in the latter [11]. These results imply that the interface structure could dictate the response of these nano-composite materials under shock loading conditions. However, since the MD studies of shock loaded bi-metal interfaces are limited, it is worthwhile to use MD to study shock and spall response of other bimetal interfaces with different properties.

In this work, we study two different bimetal interfaces between Cu and Pb. This study probes the importance of the interface structure between Cu and Pb on the selection of void nucleation sites. The remainder of this paper is organized as follows. The next Section discusses the details of the simulations undertaken in this study. The results and conclusions are presented in Sections III and IV, respectively.

COMPUTATIONAL METHODOLOGY

All of the MD simulations are based on an embedded-atom method (EAM) interatomic potential model for Cu-Pb developed by Hoyt et al [12]. This EAM potential was developed from existing EAM potentials for pure Cu [13] and Pb [14] by fitting the cross interactions to reproduce the enthalpy of mixing as a function of composition. The melting temperatures for pure Cu and Pb have been calculated to be 1279 and 618 K, respectively. It is important to note, that the Hugoniot Equation of state (EOS) calculated using this potential, for single crystal Pb, is different than the experiment [15] (refer Fig. 1) and eventually results in a solid-liquid phase transition for Pb at 90 GPa in comparison to 55 GPa under shock compression [16].

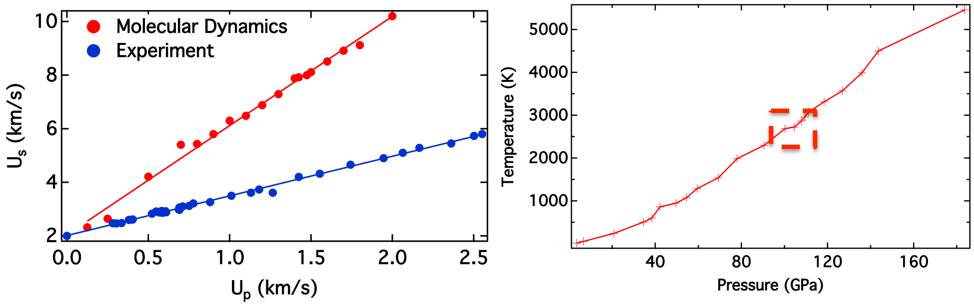

FIGURE 1. (Left) Comparison of the experimental and calculated Hugoniot Equation of State (EOS) for single crystal Pb. (Right) Calculated shock Hugoniot showing the solid-liquid phase transition using this potential under shock compression (as highlighted by the red square).

To investigate the dependence of the void nucleation on bi-metal interface orientation and structure, bi-crystal simulation cells are used. For the bi-crystals two orientation relationships (OR) between Cu and Pb are considered:

- $\{111\}_{Cu}/\{111\}_{Pb}$: $[1\ 1\ \bar{2}]_x$, $[1\ 1\ 1]_y$ and $[1\ \bar{1}\ 0]_z$.
- $\{100\}_{Cu}/\{100\}_{Pb}$: $[1\ 1\ 0]_x$, $[0\ 0\ 1]_y$ and $[1\ \bar{1}\ 0]_z$.

The MD simulations are performed using a combination of SOLVER [17] for initially relaxing the interface at 0 K and LAMMPS [18] for shock-loading simulations. The details of which can be found elsewhere [19]. The dimensions of in the x and z directions for Cu and Pb simulation layers are chosen such as to minimize the misfit strain between the two layers and ensure periodic boundary conditions. For the shock simulations, the loading direction is perpendicular to the interface and travels from Cu to Pb. The bicrystal is divided into two regions parallel to the interface plane: flyer and target. The target region is twice as long as the flyer plate and the interface is located in the center of the target at the interface between Cu and Pb (by design). Periodic boundary conditions are applied in the interface plane and the nonimpact sides of the flyer plate and target are free surfaces. The shock particle velocity is denoted by u_p and was set to 500 ms^{-1}. All shock simulations use a NVE (constant number of atoms, volume and energy) ensemble with a time step of 1 fs and total simulation times of 100 ps. To track the shock wave and other physical properties during the shock simulations, the simulation cells were divided into bins of length 5.77 Å along the shock direction. Physical properties such as particle velocity and temperature, are then averaged within each bin to give the longitudinal shock profile. The microstructural evolution is analyzed using the atomic virial stress due to the interatomic forces, assuming the zero-strain atomic volume of FCC, and centrosymmetry parameter analysis [20]. The temperature and pressure are calculated after subtracting this initial applied velocity.

RESULTS AND DISCUSSION

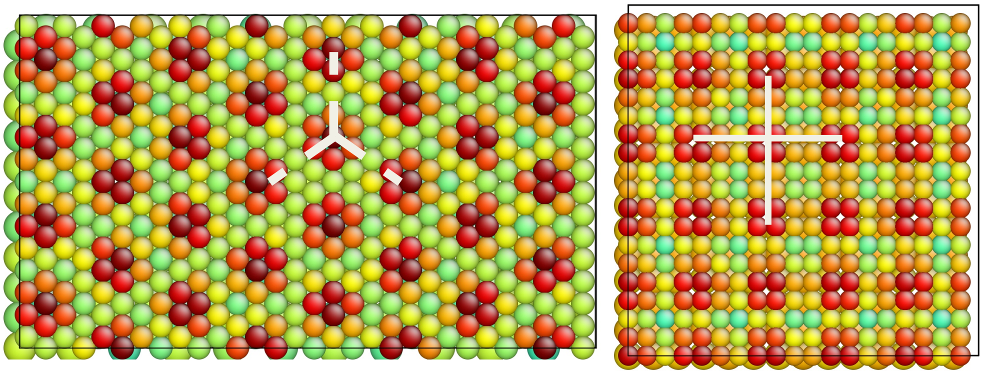

FIGURE 2. Relaxed structures for (Left) {111} and (Right) {100} CuPb interfaces at 0 K. The atoms are colored by hydrostatic stress where red represents the highest stress.

Figure 2 shows the relaxed zero temperature structures for the [100] and [111] interfaces. The interfacial free energies for these interfaces were calculated to be 0.80 J/m^2 and 0.58 J/m^2, respectively, The atoms are colored according to hydrostatic stress. These images highlight the different structure of the two interfaces, which is one of the reasons these two orientations were selected. The [111] interface is comprised of three different Shockley partials which intersect to create dislocation nodes (the red regions). In comparison, two full dislocation comprise the [100] interface and also intersect to create regions of higher stress.

The shock and spall simulations on these two interfaces show that in both the cases voids nucleate in Pb near the interface region, which retains its original structure as shown in Fig. 3. In addition, even though both cases show disordering of the Pb bi-crystal under compression near the interface, the [111] interface shows no plastic deformation in Cu at any time. The disordering in Pb is attributed to heating of the Pb crystal upon shock. It has been previously shown[16] that single crystal Pb can undergo melting under release at particle velocities of 500 ms^{-1}. In presence of Cu, additional plastic deformation in Pb from the interface could further decrease this melting temperature under release. Due to this thermal disordering of Pb, the shear strength of Pb is almost negligible and hence all voids preferentially nucleate within the Pb. These results suggest that in this case details of the interface structure do not play a major role in determining the location for void nucleation.

The response of Cu/Pb interface is different than of Cu/Nb interfaces where interface structure determined the dislocations that were emitted from the interface. This could be because the stacking fault energy in Nb is very high so only Cu can undergo plastic deformation. Whereas in the case of Cu/Pb, Pb is the softer phase and hence easier to deform. In addition, the huge difference in the melting temperatures of Cu and Pb tends to overwhelm the deformation and eventually the nucleation process. So instead of emitting individual Shockley partials under loading as observed in Cu/Cu grain boundary systems, the local increase in temperature, associated with mechanical loading of the interface dictates the response of this material. The elastic and plastic properties of both the phases together dictate if the interface structure will be important or not.

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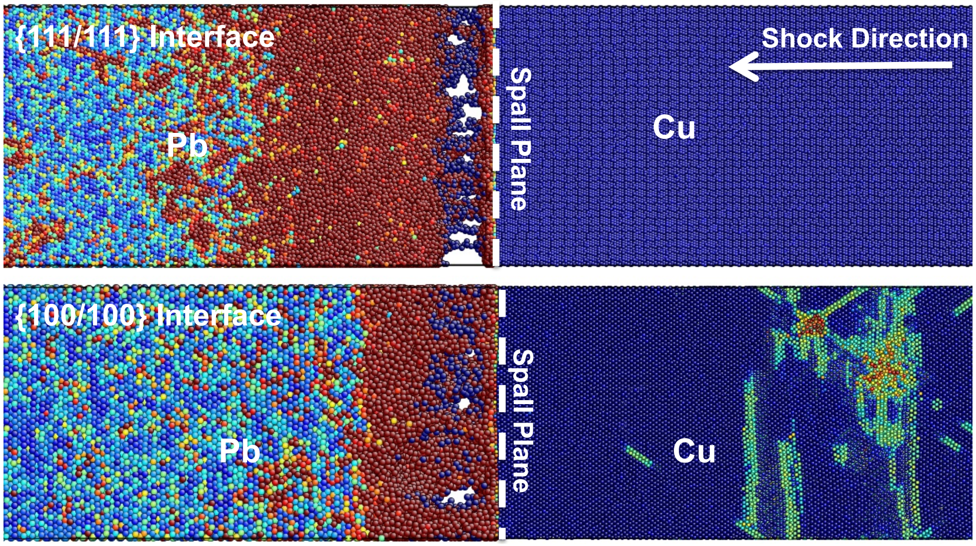

FIGURE 3. (Left) Comparison of the experimental and calculated Hugoniot Equation of State (EOS) for single crystal Pb. (Right) Calculated shock Hugoniot showing the solid-liquid phase transition using this potential under shock compression (as highlighted by the red square).

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