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The initial stage of surface modification of magnesium alloys by high intensity pulse ions beam

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ABSTRACT

The initial stage of high intensity pulsed ion beam irradiated magnesium alloys was studied by MD simulation. Specimens containing $Mg_{17}Al_{12}$ precipitation were modeled to investigate the evolution of magnesium alloys during several picoseconds after a high-energy ion impacting. It was found that the $Mg_{17}Al_{12}$ precipitation has little effects on the kinetic energy evolution in the heat zone, but considerable effects on strength of kinetic energy peak moving to the deep matrix and on the surface morphology of the magnesium alloy at thermal equilibrium state. The thickness of the heat zone is independent on the temperature of surface region.

Magnesium alloys have attracted more and more interests for their high specific strength. However, their outdoor applications are limited due to the low wear and corrosion resistance of the raw materials. Benefit to the surface modification technology, magnesium alloys with modified surface exhibit considerable improvement in wear and corrosion resistance [1–3]. High intensity pulsed ion beam (HIPIB) is a unique technology for magnesium alloys surface modification, which induces a combined improvement in wear and corrosion resistance [1]. The HIPIB technology avoids the problems and technological limitations such as limited adhesive properties [4], non-uniform deformation and residual stress [2,3], and shallow modified range [5–7]. It is a clean environmental friendship technology with rapid processing rate [8]. During HIPIB irradiation, high-intensity ions with hundreds of keV energy impact the materials surface [1]. In such energy range, effects of electronic stopping and the electron–phonon interactions will cause the lattice temperature higher than 10^7 K in the first 0.3 ps and down to 10^4 K at about 6 ps according to the simulation by Zarkadoula et al. [9]. Such high lattice temperature will produce ablation plasma with large velocity. The relationship between the kinetic energy and the temperature is

$$E = nkT = \frac{1}{2}nmv^2 \tag{1.1}$$

where E is the total kinetic energy of the ablation plasma containing n ions with mass of m. k is the Boltzmann constant, and v is the velocity of the ions. Supposing the ablation plasma was in local thermal equilibrium with the lattice at the surface region, the lattice with temperature of 10^4 K would induced the ablation plasma with velocity of 2.3 km/s. According to the numerical results of Buttapeng [10] and the experimental data obtained by Yatsui et al. [11–13], the velocity of ablation plasma caused by HIPIB was in the range of 0.7–15 km/s which is consistent with the results of electronic stopping and the electron–phonon interactions theory. For HIPIB irradiated on Mg alloys, the high lattice temperature in the initial several picoseconds will intensively change the state of irradiated magnesium alloys surface and considerably affect the following evolution. The experimental investigation on this short processing is seriously restricted by the extremely rapid processing speed. For the high spatial resolution, the molecular dynamics (MD) simulations have been extensively used to investigate the high energy density deposition process in an ultrashort time at the atomic level such as laser–material interactions [14–16]. In this paper, MD simulations of the initial stage of the HIPIB irradiation on the magnesium alloy were performed. The work focus on the materials behavior induced by an ion impacting event (IIE). The computational model and simulation procedures for the HIPIB irradiation of magnesium alloys at the atomic level are presented in the following.

The simulation boxes were constructed with dimension of 6.419 nm, 6.671 nm, and 30 nm in X, Y, and Z directions, respectively. Pure Mg crystal was prepared by filling the simulation box

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from 0 to 26.153 nm along Z direction in an h.c.p lattice with constant of 0.3209 nm as shown in Fig. 1(a). Samples with $Mg_{17}Al_{12}$ precipitation were prepared by substitute a cubic block region with length of 3.165 nm of pure Mg crystal at various depths by $Mg_{17}Al_{12}$ precipitation in Fig 1 (b)–(f). Fig. 1(g) shows the structure of $Mg_{17}Al_{12}$ precipitation. It contains 1566 atoms and has an α-Mn-type cubic unit cell (space group I43 m) with lattice parameter of 1.056 nm [17]. The MD samples depicted in Fig. 1(a)–(f) were named A–F. For samples B–F, the distance between the top interface of the $Mg_{17}Al_{12}$ precipitation and top surface of the magnesium matrix are 0, 1.5, 3.0, 4.5 and 16.5 nm, respectively. The mass center of the $Mg_{17}Al_{12}$ precipitation were at $X = 3.209$ nm, $Y = 3.336$ nm for all magnesium samples. Periodic boundary conditions were imposed in X and Y directions. The free boundary condition in Z direction was used to avoid the reflection effect caused by using fixed or period boundary conditions. The rigid motion of the specimen was restricted by the bottom surface atoms through setting the force zero. The atomic interactions in the magnesium alloy specimen were described by Finnis–Sinclair embedded-atom method (potential #4 in Ref. [18]). Because $Mg_{17}Al_{12}$ phase has a different lattice structure with the magnesium matrix, artificial high local stress could appear near the interface of the precipitation and the magnesium matrix. To eliminate the artificial high local stress of the samples with $Mg_{17}Al_{12}$ precipitation, the Polak–Ribiere version of the conjugate gradient (CG) algorithm was employed to carry out an energy minimizing procedure for samples B–F. Then, Samples A–F were relaxed at 300 K and 0 bar for 15 ps within isothermal–isobaric NPT ensemble (Nose–Hoover thermostat) to its equilibrium configuration. The positions of all atoms in specimen were stored for the following simulations. The lattice temperature T_s of the surface region with thickness of 1.048 nm were assigned a value in the range of 2×10^4–1.8×10^5 K at 0 ps to simulate the effect of IEE. The simulations of HIPIB irradiation procedure were achieved within microcanonical NVE ensemble for 3 ns which is long enough in our simulation. OVITO code [19] was used to visualize and analysis

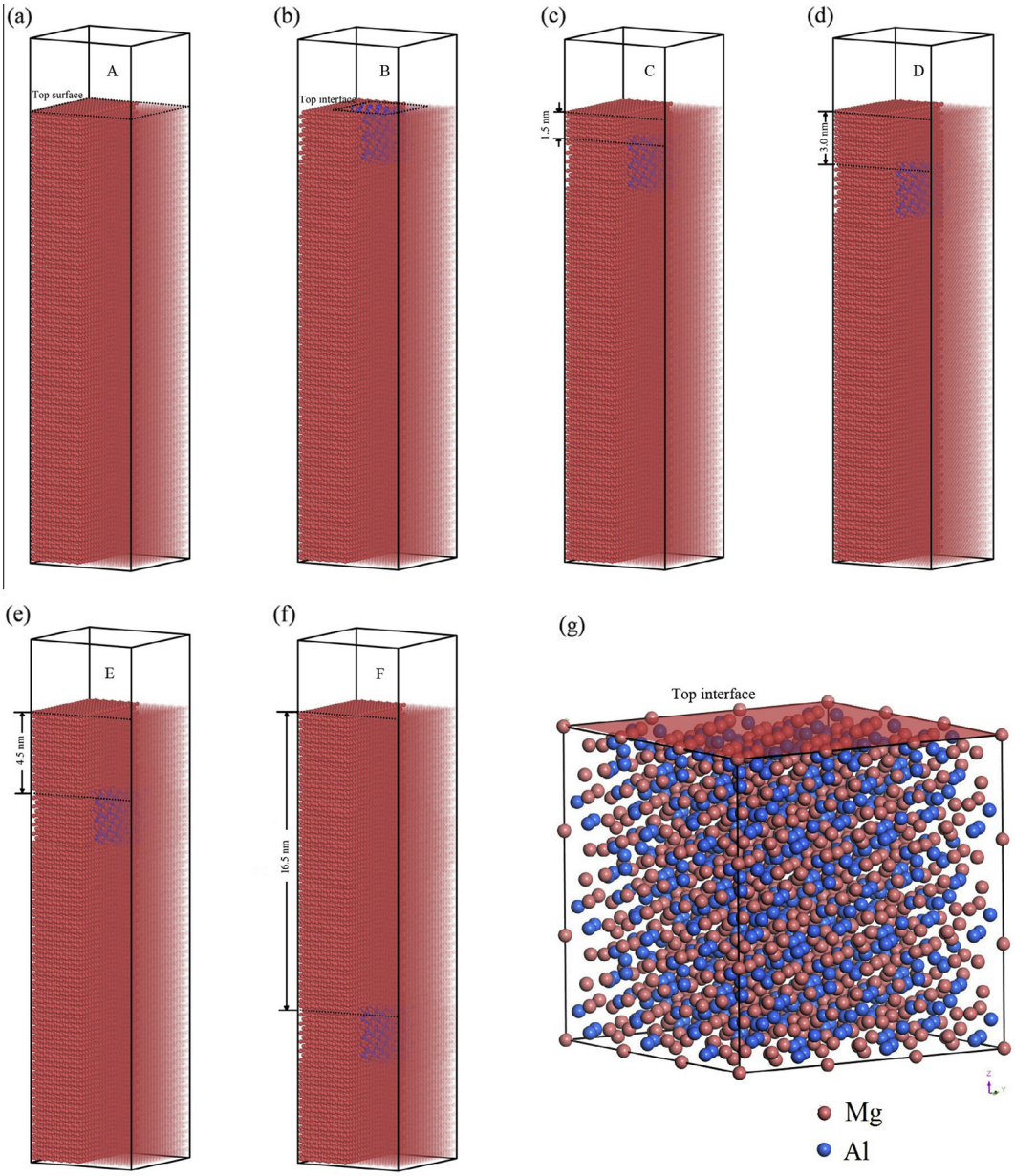

Fig. 1. The MD samples of HIPIB irradiation on the magnesium alloy surface utilized in current study.