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Influence of high-intensity pulsed ion beam irradiation energy on magnesium alloy surface modification

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ABSTRACT

Magnesium alloys surface modified by high-intensity pulsed ion beam irradiation are studied by MD simulation. The specimens containing defects were modeled to investigate the effect of high-intensity pulsed ion beam irradiation on surface area and defect size. It was found that the surface area mainly depend on the value of irradiation energy. The kinds of defects in the sub-surface have little influence on the surface area. The inner surface of the defect decreases with the increasing irradiation energy. There was a nonlinear relationship between the irradiation energy and the defect size.

Magnesium alloys are being considered as promising structural materials for industrial application due to the attractive properties, such as low density, high strength-to weight ratio, high dimensional stability and good machinability etc. Poor wear and corrosion resistance restricts their application, even in outdoor application. A number of surface engineering methods, including physical and chemical methods, have been developed to improve the wear and corrosion resistance of magnesium alloys. However, Chemical methods such as chemical conversion coating [1], anodizing [2] and plating [3] has to use the toxic precursors which may cause a serious of environmental pollution problems. The physical approaches such as physical vapor deposition of thin films [4], laser surface melting [5], alloying [6] and conventional ion implantation using a series of gas/metal ions [7–9] are also confronted with the technological limitations, e.g. limited adhesive properties, non-uniform deformation and residual stress, and shallow modified range etc. To avoiding the problems and technological limitations mentioned above, high-intensity pulsed ion beam (HIPIB) is a unique technology [10], and has been developed as a powerful tool for the surface modification of magnesium alloys [11,12]. In our previous work, HIPIB irradiation of magnesium alloy is performed. The combined improvement in wear and corrosion resistance of AZ31 magnesium alloy is achieved by HIPIB irradiation due to the microstructural refinement and the chemical homogeneity based on annihilation of defects [12].

During HIPIB irradiation, ignorable irradiation dose (4–12 ions/cm^2) of carbon and hydrogen atoms was implanted into the target materials. High energy density deposition into a shallow range within an ultrashort time pulse duration in a rapid melt or evaporation of near surface layer of materials with extremely heating rates typical of 10^8–10^{11} K/s. Giving the resolution limitation of measuring apparatus, experimental investigation of the HIPIB irradiation effect on the surface modification is seriously restricted due to the ultrashort time of pulse duration. On the theoretical side, the molecular dynamics (MD) simulation has been extensively used to investigate the high energy density deposition process in an ultrashort time such as laser-material interactions at the atomic level for its high spatial resolution [13–15].

Previous studies mainly focused on the temperature field in the region near the surface during pulsed ion beam irradiation by finite element method [16]. The finite element method can describe the melting and re-solidification processes very efficiently. However, the macroscopic method neglects the effect of defect at atomic level. Therefore it is hard to explain the improvement of corrosion resistance of the magnesium alloys after irradiation. In this paper, MD simulations of the HIPIB irradiation on the magnesium alloy surface were performed, with focus on the processes of defect annihilation in the surface under a huge temperature gradient. The

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computational model and simulation procedures for the HIPIB irradiation of magnesium alloys at the atomic level are presented.

The MD model of HIPIB irradiation on the magnesium alloy surface utilized in current study consists of a magnesium alloy specimen under HIPIB irradiation field, as depicted in Fig. 1. The magnesium alloy lattice is hcp lattice with lattice constant of 0.3209 nm. The simulation box of specimen has a dimension of 3.209 nm, 5.558 nm, and 20.960 nm in X, Y, and Z direction, respectively. The specimen has a dimension of 3.209 nm, 5.558 nm, and 18.340 nm in X, Y, and Z direction, respectively containing 14,200 atomic positions. Periodic boundary condition is only imposed in X and Y directions. To simulate the behavior of defects under the condition of HIPIB irradiation at atomic level, a sphere region with radius of 0.642 nm, block regions A and B with dimension of 3.209 nm $\times$ 1.112 nm $\times$ 5.240 nm and 3.209 nm $\times$ 1.112 nm $\times$ 10.480 nm were deleted from the specimen, respectively, to make a sphere-shape defect and micro crack defects. The mass center of the sphere, block-shape A and block-shape B were at (1.605 nm, 2.779 nm, 14.642 nm), (1.605 nm, 2.779 nm, 18.864 nm), and (1.605 nm, 2.779 nm, 12.052 nm). It is seen from Fig. 1 that the specimen contains two kinds of atom positions, as boundary atom position, and Newtonian atom position, respectively. All these positions were filled by Mg atoms and Al atoms with possibility of 96.9 at% and 3.1 at%, which represents the composition of AZ31. The rigid motion of the specimen is restricted by the boundary atoms through setting the force zero. The atomic interactions in the magnesium alloy specimen are described by Finnis–Sinclair embedded-atom method [17]. To eliminate the high potential energy and high local stress associated with the improper atoms in defect region, the as-prepared magnesium alloy specimen is relaxed within isothermal-isobaric NPT ensemble (Nose-Hoover thermostat) to its equilibrium configuration by following procedures: the specimen is equilibrated at 300 K and 0 bar for 15 ps. The positions of all atoms in specimen were stored for the following simulations.

In this work, the simulations of HIPIB irradiation are achieved within microcanonical NVE ensemble by LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) code [18]. For the limited calculation ability, we only study the process during a heat shock passing through the defect. The specimen with Newtonian atoms consistent of two part: the part in the surface region with thickness of 1.048 nm containing 1000 atoms. The velocities of the atoms in this region were assigned Gaussian-type distribution. After the energy were assigned, the Newtonian atoms in the magnesium alloy specimen are relaxed within NVE ensemble for 150 ps, which was observed long enough to get equilibrium state. OVITO code [19] was used to quantitative measure the outer and inner surfaces area of the magnesium alloy. The probe sphere radius and smoothing level were set to 4 nm and 8, respectively.

Fig. 2 gives the equilibrium states topographies of the magnesium alloy specimens containing (a) no defect, (b) a sphere-shape defect, (c) a block-shape defect A, (d) a block-shape defect B in the subsurface after 150 ps with irradiation energy of 6000 eV (5.3×10^{-2} J/cm^2) from HIPIB irradiation. The gray scale indicates the distance of the atom from the paper plane, the white color means a shorter distance of the atom from the paper plane. It was shown that the surface roughness of all specimens increased slight after the irradiation. The area of the surface increased from 17.84 nm^2 to 18.82 nm^2, 19.77 nm^2, and 19.47 nm^2 for the specimen in Fig. 2(a–d). It also be noted that cracks appeared in the specimens containing no defect and a sphere-shape defect. And there were no cracks in the specimens containing block-shape defects A and B. The cracks may be caused by the intensely shock wave induced by thermo effect of HIPIB irradiation. And in the specimens with block-shape defects, the energy of shock wave was exhausted or minimized by annihilation of the block-shape defect. It suggested that the volume of cracks parallel to the irradiation direction will be reduced while the perpendicular one will get increased. All the defects vanished after 150 ps except the block-shape defect B which is too large for the case of irradiation energy being 6000 eV.

To study the effect of irradiation energy on the defect annihilation, the specimen containing a block-shape defect B was chosen. All simulation parameters were the same as the case in Fig. 2, except the irradiation energy. In the following simulation, the energy was modified in a range from 500 eV to 6000 eV instead of constant value 6000 eV. Fig. 3 gives the equilibrium states topographies of the magnesium alloy specimens containing a block-shape defect B after 150 ps since obtaining 500 eV (4.4×10^{-3} J/cm^2) to 6000 eV (5.3×10^{-2} J/cm^2) from HIPIB irradiation. The

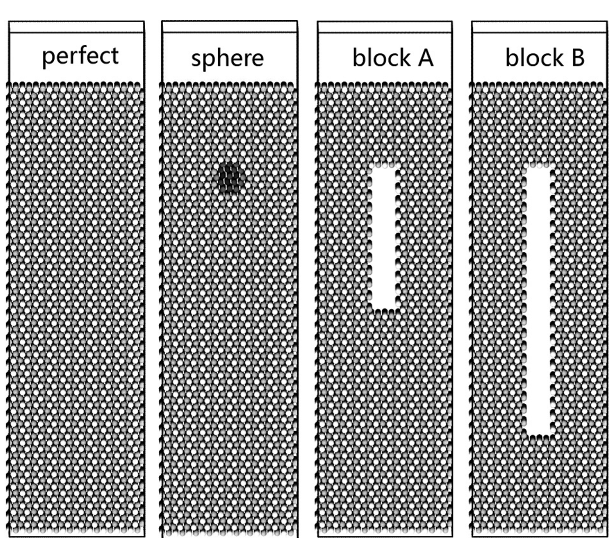

Fig. 1. Model of magnesium alloy specimen under HIPIB irradiation field.

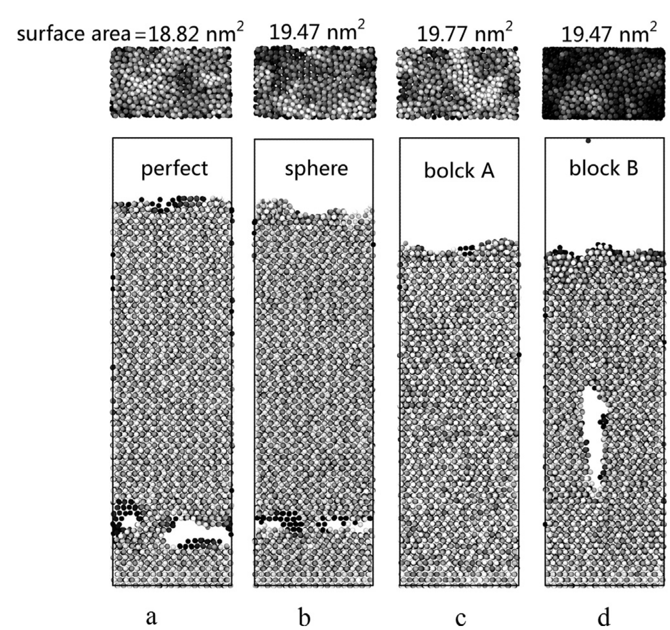

Fig. 2. The equilibrium states topographies of the magnesium alloy specimens containing (a) no defect, (b) a sphere-shape defect, (c) a block-shape defect A, (d) a block-shape defect B in the subsurface after 150 ps with irradiation energy of 6000 eV from HIPIB irradiation.