ATOMISTIC SIMULATION OF COMPRESSION DEFORMATION BEHAVIOR IN MAGNESIUM SINGLE CRYSTAL

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Summary In our molecular dynamics simulation, shearing due to a successive slip of $\{11\bar{2}2\}$ planes along the $\langle 11\bar{2}\bar{3}\rangle$ direction is responsible for the deformation under the c-axis compression at the nanoscale. The full pyramidal slip of $\frac{1}{3}(\bar{1}\bar{1}22)[\bar{1}\bar{1}2\bar{3}]$ ($\pi 2$) is accomplished by two steps, the first step is a $\frac{1}{6}[20\bar{2}\bar{3}]$ slip, and then followed by a $\frac{1}{6}[02\bar{2}\bar{3}]$ slip. Between these two steps, the stacking fault forms.

Magnesium alloys have attracted attention in recent years as lightweight materials for the transportation industry due to their low density and relatively high specific strength. However, the application of magnesium alloys is restricted due to the limited forming capacity and the poor corrosion resistance. From the mechanical point of view, magnesium and its wrought alloys show a pronounced direction-dependence of plastic yielding and work hardening, as well as different yielding behavior in tension and compression, the so-called strength differential (SD) effect [1]. This feature is due to the crystal structure of magnesium, which is a hexagonally close-packed (hcp) structure. Compared to face-centered cubic (fcc) or body-centered cubic (bcc) metals, the number of slip systems allowing plastic deformation in magnesium is limited. As a consequence, the material deforms by twinning, which is usually regarded as the dominant deformation mode.

In previous paper, the deformation behavior in magnesium single crystal under c-axis tension was investigated by molecular dynamics simulations [2]. At a low temperature, twinning was found to be the main deformation mechanisms. In particular, the $\{10\bar{1}2\}$ tension twins with the reorientation angle of about 90° were observed in the simulations. Grain nucleation and growth are found to be accompanied with the $\{10\bar{1}2\}$ twinning. It is noteworthy that both the $\{10\bar{1}2\}$ ($\pi 3$) tension and $\{10\bar{1}1\}$ ($\pi 1$) compression twinning were observed in this simulation of c-axis tension.

In this paper, the deformation behaviors in magnesium single crystal under the c-axis compression at different temperatures are investigated by molecular dynamics simulations. A plane strain condition was considered in order to reduce the computational cost compared to a full 3D simulation, with a periodic boundary condition applied in the $[\bar{1}2\bar{1}0]$ direction. Initial configurations of Magnesium single crystal samples are first defined in the simulations. At the top of the model, four layers of atoms were frozen and then given a stepwise displacement along $[000\bar{1}]$ direction in order to create a compression load. Between each small displacement, all atoms were relaxed for certain number of steps of magnitude 6×10E-15s with the fixed-displacement boundary condition, and the evolution of atomic positions in the crystals at different loading levels was investigated. Isothermal−isobaric ensemble was employed and the temperature of the system was kept relatively constant during the simulation. An EAM potential for Magnesium developed by fitting both the ab initio forces and experimental data on various bulk structural properties is applied [3]. The Classical molecular dynamics code Lammps [4] was used for the atomistic simulations

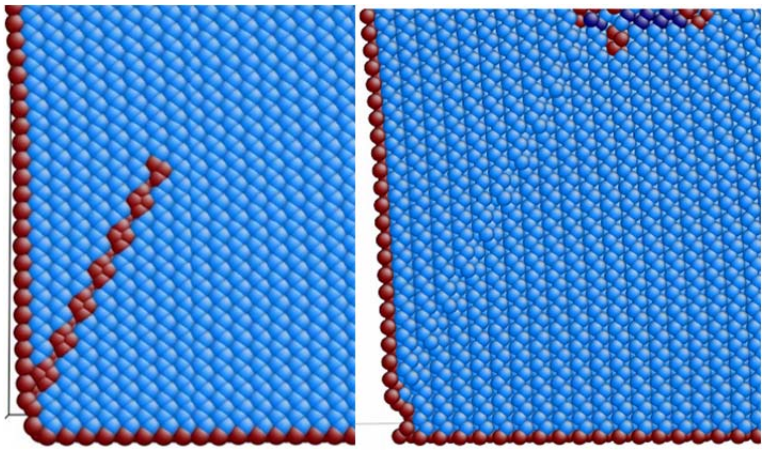

Figure 1: (a) A stacking fault forms after the slip of $\frac{1}{6}[20\bar{2}\bar{3}]$; (b) A full pyramidal slip of $\frac{1}{3}(\bar{1}\bar{1}22)[\bar{1}\bar{1}2\bar{3}]$ ($\pi 2$) is finished after the subsequently slip of $\frac{1}{6}[02\bar{2}\bar{3}]$.

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Simulations under c-axis compression show that the pyramidal $\{11\bar{2}2\}$ slip dominates under compression loading. No compression twins are observed at different temperatures for different loading and boundary conditions. We have carefully examined the stepwise dynamic response of the deformation, and observed the nucleation of dislocations at the free surface and at the interior defect, separately. It is found that a full pyramidal slip of $\frac{1}{3}(\bar{1}\bar{1}22)[\bar{1}\bar{1}2\bar{3}]$ ($\pi 2$) is accomplished by two steps, the first step is a $\frac{1}{6}[20\bar{2}\bar{3}]$ slip, and then followed by a $\frac{1}{6}[02\bar{2}\bar{3}]$ slip. After the first step of a $\frac{1}{6}[20\bar{2}\bar{3}](30\bar{3}4)$ slip, a stacking fault is formed as shown in Fig. 1(a). Only when the second step is accomplished, a full pyramidal slip of $\frac{1}{3}(\bar{1}\bar{1}22)[\bar{1}\bar{1}23]$ ($\pi 2$) can be finished as shown in Fig. 1(b). Thus a full pyramidal slip of $\frac{1}{3}(\bar{1}\bar{1}22)[\bar{1}\bar{1}23]$ ($\pi 2$) can be expressed as

$$\frac{1}{3}[11\bar{2}\bar{3}] \rightarrow \frac{1}{6}[20\bar{2}\bar{3}] + \frac{1}{6}[02\bar{2}\bar{3}].$$

In this simulation, shearing due to a successive slip of $\{11\bar{2}2\}$ planes along the $\langle 11\bar{2}\bar{3}\rangle$ direction is responsible for the deformation under the c-axis compression. No twinning with symmetrical structure has been found. A slip step appears at the surface of the sample after the slip moves out of the sample. Meanwhile, some interior defects are also left behind at the end of the shear region. This result is exactly consistent with the microcompression measurements of single crystal magnesium that no twinning was observed in sample sizes from 2.1 to 10 μm under c-axis compression, and significant plasticity and hardening occurred due to six active pyramidal slip systems [5, 6].

References

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