Analysis and Nanomold Design for Aluminum Nanoimprinting

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A nano-forging process based on the potential function of an embedded atom method (EAM) and mechanism, for pure aluminum samples, was studied using molecular dynamic (MD) simulation. The effects of forging temperature and velocity were evaluated in terms of molecular trajectory, internal energy, and a radial distribution function. The simulation results clearly show that the internal energy exerted by the workpiece during the forging process rises with a decrease of forging temperature, and an increase of forging velocity also raises the internal energy. During the forging process, a special atomic structure in the (011) and (0 1 1) slip planes was observed that represents the site of dislocation generation and growth nucleation. When severe plastic deformation occurs, the density of the workpiece changes. The forged workpiece has similar distributions of atomic density after loading at different forging temperatures and velocities.

1. Introduction

Technology in modern production has progressed in a highly precision-oriented direction and some has even reached nanometer-scale microstructure. The development of nanofabrication technology includes top-down approaches such as photolithography [1] and maskless lithography [2]. Nanofabrication based on mechanical processes also has very wide application in semiconductor devices in combination with electronic, mechanical and optical technology on a single substrate. Photolithography uses light to transfer a geometric pattern from a photo mask to the substrate. Maskless lithography, can also be used in precise nanofabrication, where laser light, an electron or and ion beam, or even physical pressure from a mechanical device can be used to alter the nanostructure of a substrate. Among these, nanoimprinting or nanoforming lithography applications have been demonstrated as useful to nanoscale size [3].

Molecular dynamics (MD) can be used to effectively describe the mechanism of surface material structure at nanometer scale. The fundamental theory is derived from Newtonian mechanics and integral equations are combined with computer programs to calculate the trajectory between atoms and molecules. Many nano-scale studies have been conducted using MD, such as those involving surface friction [4], scratching [5], imprinting [6], and nano-indentation [7].

Forging is a manufacturing process where compressive forces are used to shape a soft material into a desired pattern. Aluminum is one of the important metals used in such applications [8]. In this study, the effects of forging temperature and velocity on the mechanical properties of aluminum samples during the nanoforging process are studied using MD simulation. The results are discussed in terms of molecular trajectories, energy, and radial distribution function.

2. Method

Molecular dynamics was used in this study to simulate metal forming by nano forging. Fig. 1 shows the simulated model. A slug of pure monocrystalline aluminum was created and placed in the fixed end of a die. The punch was fixed to the other end of the aluminum slug, it was given a speed to implement closed-die forming of the aluminum inside the die. The material of the die and punch was nickel (Ni). The aluminum and nickel atoms were both arranged in a perfect FCC lattice structure. The size of the cavity in the die was 3.0(X-)*10.5(Y-)*2.1(Z-)nm and the punch was 3.0(X-)*14.7(Y-)*1.2(Z-)nm. The aluminum slug was 3.0(X-)*4.2(Y-)*9.9(Z-)nm. The die and punch were set as fixed layers, and the aluminum was set as a free atom layer. The X-direction was given the condition of a periodic boundary.

In this study the nanoforming process was simulated under forging temperatures between 275 and 710K and speeds of between 30 and 100m/s. Th potential energy of the forged piece (Al-Al) and forged piece and the die (Al-Ni) atomic action mechanism has been described using the EAM potential energy deduced by Daw and Baskes [9] from the density functional theory of quantum mechanics.
EAM is the abbreviation used for "embed atom method", suggesting that the energy is formed from embedding atoms in other atomic lattice groups. The potential energy is described by cloud density. The total energy \( E \) of the atomic system using this method is expressed as \([9]\):

\[
E = \frac{1}{2} \sum_{i,j} \phi_{ij}(\rho_i) + \sum_i F_i(\rho_i)
\]  

(1)

where \( \phi_{ij} \) is the acting force between Atom i and Atom j, and is two-body potential, \( F_i \) is the energy of embedding atoms in other atomic lattice groups, the cloud density is the required energy for the region of \( \rho_i \), and is expressed as:

\[
\rho_i = \sum_{j \neq i} f_j(\rho_j)
\]  

(2)

where \( f(\rho_i) \) is the electron density function, a many-body term. The two-body potential and charge density are expressed as Eqs. (3) and (4).

\[
\phi(r) = \frac{A \exp \left[ -\frac{c}{(r - \alpha)} \right] - B \exp \left[ -\frac{d}{(r - \beta)} \right]}{1 + \frac{c}{(r - \alpha)}}
\]  

(3)

\[
f(r) = \frac{f_c \exp \left[ -\frac{\beta}{(r - \lambda)} \right]}{1 + \frac{\beta}{(r - \lambda)}}
\]  

(4)

The parameters for this potential energy are shown in Table 1 [9]:

|     | \( r_c \) | \( f_c \) | \( \rho_c \) | \( \alpha \) | \( \beta \) |
|-----|----------|----------|-------------|-----------|-----------|
| Ni  | 2.488746 | 2.007018 | 27.984706   | 8.029633  | 4.28247   |
| Al  | 2.886166 | 1.392302 | 20.226537   | 6.942419  | 3.70262   |
| A   | 0.439664 | 0.652771 | 0.413436    | 0.826873  |           |
| B   | 0.251519 | 0.313394 | 0.395132    | 0.790264  |           |

3. Results and discussion

3.1 Deformation of nanoforging

Fig. 2 is the schematic diagram of the nanoforging deformation mechanism when the temperature is 400K and the pressing speed of the punch is 30m/s. Figs. 2a-d show the deformation mechanism of material at different punch pressures and 2e-h show holding and unloading. An internal energy field is used to express the increase and decrease in the energy resulting from the forming of atoms under pressure and the internal energy is the sum of kinetic and potential energy.

As can be seen from Fig. 2a, the higher internal energy values occur in the contact surfaces between the aluminum slug and the punch and die. These regions have larger loading capacity. When the punch applies an external acting force to the aluminum it is compressed so that free atoms flow toward unconstrained space. As the punch continues to press, more free atoms are subject to pressure so that the aluminum deforms until the entire die cavity is filled.

When the metal is moved by an external force, dislocation results in flow of metal in the shear direction. Figs. 2b and 2c show the slip direction of dislocation and the formation of grain boundaries, and (011) and the (011) slip plane and slip bands can be observed in the atomic structure. A significant amount of relatively high deformation energy is dispersed over this region. The internal energy of the material reaches its maximum until the die is closed. This usually occurs in the region next to the punch, as shown in Fig. 2d, suggesting that the interatomic distance is very short in this region and at this time. The repulsive energy is relatively strong, so that the energy is higher and will be balanced for a period.

The energy can be mitigated by holding, as shown in Fig. 2e and a decrease of energy in the region next to the punch can be observed. Fig. 2f-h shows the unloading process. In the microscopic domain, the size changes result in strong viscous forces between the material and the punch and die. This study used higher unloading speed to...
reduce the viscous effect, and the demolding is assumed to be perfect.

3.2 Forging temperature effect

The simulated forging temperature region used was between 275 and 710K. Forging at room temperature was regarded as cold forging and temperatures higher than the recrystallization temperature of the material were regarded as hot forging process. Fig. 3 shows the variation of the energy of the aluminum at different forging temperatures with punch loading, holding and unloading, and the energy is negative, meaning the atoms are mostly in a viscous state. This is because the atoms are not constrained at all in the original state, and the energy is stable by free heat balance. At depths of 0.5 to 4nm, the punch has contacted the surface of the aluminum slug. Micro-deformation has started so that the energy has increased slightly and then it increases sharply as the pressing depth becomes greater, this suggests that a higher load will cause more plastic deformation. The state is closed until pressing depth reaches 5.43nm, and energy reaches the maximum. In terms of forging temperature, the energy value at low temperature is larger than that of the environment at high temperature, this is because plastic flow of the Al is relatively easy at a higher forging temperature.

The die is given holding, and in the Fig. it can be seen that the energy decreases gradually as holding time increases. This is because holding helps the atoms in the relatively dense region near the punch to rearrange themselves in appropriate positions, so that energy is balanced and stress distribution in the aluminum becomes relatively uniform. In the final unloading stage, the energy decreases slightly as the punch rises, because the atoms migrate towards free space during unloading, the energy is released, and the atoms attract each other, but the downtrend was small in this study to reduce the viscous effect.

3.3 Forging speed effect

Fig. 5 is a diagram of the internal energy field in the closed state at 400K with a punch speed range of between 30 and 100m/s. It is clear that the region of high internal energy is more significant as the punch speed increases, and the atoms are clustered mainly in the region closest to the punch. Fig. 6 shows the variation of energy with an increase of pressing depth at different punch speeds. It can be seen that the energy value is greater when the punch speed is high, because the heavy impact of the punch on the atoms results in a more even application of force. There is also insufficient time for recovery or adjustment of dislocations and stacking faults in the material.

3.4 Analysis of the radial distribution function (RDF) of forging temperature and speed

The RDF describes the distribution probability of other atoms within the radius of one specific atom. Fig. 7 shows the variance in RDF for four different punch depths (D) at 400K and a punch speed of 30m/s. At a depth of 0.0nm, the punch has not yet applied pressure to the material after heat balance. The aluminum material has perfect face-centered cubic lattice structure, the radius of the maximum peak is 0.28nm, which suggests that the aluminum atoms have smaller energy within this radius. When the pressing depth reaches 1.9nm, the peak value decreases, as the load increases when the die cavity is about to be filled. When the pressing depth reaches 3.7nm, the height of the peak decreases slowly, and the radius decreases to 0.27nm.
Finally, when the pressing depth has reached 5.4nm, the die is completely closed and the main peak shows a large change. The dense atoms are compressed in the die cavity and are in a constrained space. The distance between atoms is reduced so much that the radius of the maximum peak decreases to 0.24nm.

Figs. 8 and 9 describe the RDF of the aluminum material in the closed state when the pressing depth is 5.43nm at different forging temperatures and punch pressing speeds. The kinetic energy increases with the temperature, but according to Fig. 8, there is no significant difference in the trend of RDF, because the atoms are constrained in the die cavity. When the die cavity is full the free space for atom flow becomes very small.

Fig. 5 Loading state at 400K and forging speeds of (a) 30, (b) 40, (c) 50, (d) 60, (e) 70, (f) 80, (g) 90, (h) 100 m/s

Fig. 6 The relationship between energy and pressing depth at different punch speeds

Fig. 7 Variation of RDF with pressing depth (D) at 400K and a punch speed of 30m/s.

4. Conclusion

This study analyzed the nanoforging process using molecular dynamics and the conclusions are as follows.
In the forging process, the atomic structure of the workpiece shows dislocation slip because of defects, the slip planes are $(0\overline{1}1)$ and $(0\overline{1}1)$, and the atoms located near the slip planes will have higher energy.

The energy value of the atomic structure of the workpiece decreases relatively as the forging temperature increases.

The internal energy and pressure values of the atomic structure of the workpiece increase with punch speed.

When the forging temperature and punch speed are changed, as confined to the die, there is only slight difference in the density of the interatomic structure of workpiece in the loading state.

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