Interface-governed nanometric machining behaviour of Cu/Ag bilayers using molecular dynamics simulation

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The nanometric machining of Cu/Ag bilayers and pure Cu film is performed using molecular dynamics (MD) simulations. The mechanical and tribological properties of Cu/Ag bilayers are investigated by comparing with those of pure Cu film. The effects of machining parameters (indenter radius, tool speed and machining depth) on the subsurface damage and material removal are studied by analyzing the dislocation movement, chipping volume, machining force and average temperature of the workpiece. The results show that the hardness of Cu/Ag bilayers is smaller than that of pure Cu film, due to the dislocation nucleation and emission from the Cu/Ag interface. Meanwhile, the friction coefficient of Cu/Ag bilayers is larger than that of pure Cu film. Furthermore, the metal bonding energy at the Cu/Ag interface is weaker than that in pure Cu film, which causes the low hardness in the Cu/Ag bilayers. The Young’s moduli in the Cu/Ag bilayers and pure Cu film are calculated by the Hertz contact mechanism and are close to the experimental result. During nanometric machining of Cu/Ag bilayers, the larger indenter radius or higher tool speed would cause a larger indentation force. The chipping volume, machining force and average temperature would increase with the increment of indenter radius, tool speed and machining depth. The subsurface damage can be reduced by selecting the smaller indenter radius, lower tool speed, and smaller machining depth, where fewer lattice defects are produced. In addition, the selection of lower tool speed also plays a crucial role in improving the smoothness of the ground surface.

1. Introduction

Nanoscale bilayer materials possess high strength,\textsuperscript{1–3} good stability and ductility,\textsuperscript{4,5} and strong fracture toughness,\textsuperscript{6} which demonstrates their great potential application as hard coatings, in aerospace equipment, X-ray optics and nano-electro-mechanical systems (NEMS).\textsuperscript{7–11} However, nanoscale bilayer materials are routinely underutilized because of high machining cost and lower machining efficiency. Thus the deformation behaviors as property indicators are fully analyzed to further understand the machining of these materials in the nanoscale level,\textsuperscript{12–15} thereby improving the machining properties and efficiency. Experimental observation often has the features of uncertain measurements, high costs and long time durations.\textsuperscript{16,17} Therefore, MD simulation is applied to track the deformation dynamics, identify the defect structure and reveal the deformation mechanism in nanoscale bilayer or polycrystal materials.\textsuperscript{18,19} A number of MD simulation studies have provided valuable insights into the ultra-precision machining of bilayers. For example, Cao et al. investigated the mechanical and tribological properties of Ni/Al bilayers.\textsuperscript{20} Shao et al. explored the dislocation–interface interaction during nanoindentation of Cu/Ni bilayers.\textsuperscript{21} Fang et al. revealed the nanoindentation mechanisms and mechanical responses of Al/Ni bilayered films.\textsuperscript{22} Cheng et al. studied the effect of misfit dislocations on the tribological behavior of Cu/Ni bilayers.\textsuperscript{23} Although the above studies are important for us to promote understanding of the deformation behaviors and properties in metal bilayers, the Cu/Ag bilayer materials are regrettably little-studied at the nanoscale. Cu/Ag bilayer materials are commonly used in engineering fields because of their strong anti-oxidation properties, good electrical and thermal conductivity, and high strength.\textsuperscript{22–24} According to the actual physical system mentioned in the experiment of Cu/Ag multilayers,\textsuperscript{24} the model of Cu/Ag bilayers is built in the current simulation to investigate the interface-governed nanometric machining behaviour for Cu/Ag bilayers. In addition, as the Cu and Ag metals are current-carriers, the electrical conductivity of Cu/Ag alloy is weaker than that of the Cu/Ag bilayers. Hence, the current Cu/Ag model is set as a bilayer system. The nanoindentation of Cu/Ag bilayers had been conducted by MD simulations to clarify the plastic deformation mechanism controlled by Cu/Ag interface in our previous work,\textsuperscript{25} but the effect of Cu/Ag interface on the
mechanical and tribological properties, including hardness and friction coefficient, as well as the subsurface damage and material removal during the nanometric machining of Cu/Ag bilayers with the various machining parameters have not been studied detailedly so far.

Therefore, in this paper, MD simulations are conducted to investigate the mechanical and tribological properties of Cu/Ag bilayers during nanometric machining. The indentation force, Young’s modulus, indentation hardness, and friction coefficient of Cu/Ag bilayers are investigated by comparing with those of pure Cu film. In addition, the effects of machining parameters on the subsurface damage and material removal are discussed via analyzing the dislocation movement, chipping volume, machining force and average temperature of workpiece. The MD simulations are helpful to understand the effect of interface on the mechanical and tribological properties and the machining properties of bilayer material from atomic level, which is beneficial for developing ultra-precision machining of bilayer materials.

2. Simulation method

Fig. 1 shows the MD simulation model for nanometric machining of Cu/Ag bilayers. The model comprises a rigid diamond tool and a workpiece of Cu/Ag bilayers. In order to reveal the interface effect on the mechanical andtribological properties of Cu/Ag bilayers, the pure Cu film with the same dimension is introduced as a workpiece for nanometric machining. Table 1 gives simulation parameters of the Cu/Ag bilayers, pure Cu film and tool. The diamond tool has a spherical shape with selected radii of 3.0 nm, 4.0 nm and 5.0 nm. The tool is seen as a rigid body in the simulations because the stiffness of diamond is far larger than that of Cu or Ag metals.

The Cu/Ag bilayers consist of Ag substrate and Cu thin film. The Ag substrate with three orientations of x-[1 0 0], y-[0 1 0] and z-[0 0 1] has a size of 14 nm × 22 nm × 6 nm. The Cu thin film with a layer thickness of 3 nm is bonded to the top of Ag substrate. The three orientations of Cu thin film are in x-[1 0 0], y-[0 1 0] and z-[0 0 1], respectively. The size of pure Cu film is 14 nm × 22 nm × 9 nm, and x-[1 0 0], y-[0 1 0] and z-[0 0 1] are three orientations of the pure Cu film. The nanometric machining is conducted along [0 1 0] direction on (0 0 1) surface of workpiece. Both x and y directions are set as the periodic boundary conditions to avoid the effect of simulation length-scale. The positive direction of z-axis is defined to be free because the (001) surface of workpiece is machined. There are three types of atoms in the workpiece: Newtonian atoms, thermostat atoms and boundary atoms. The boundary atoms are fixed to prevent the rigid body motion of workpiece. The slip behavior between Cu film and Ag substrate is ignored as the slip speed is far slower than the speed of dislocation motion, and the machining distance is shorter during the nanometric machining. The thermostat atoms are set to carry out the dissipation of heat generated the nanometric machining. The motion of Newtonian and thermostat atoms follows classical Newton’s second law whose motion equations are integrated by the velocity-Verlet numerical integration algorithm. The initial temperature of workpiece is set as 293 K. The initial velocity of atoms is assigned on account of Maxwell–Boltzman distribution. During the MD simulation process, the average temperature of workpiece is calculated from the equation:

\[ T = \left( \frac{\sum_{i=1}^{N} m_{i}v_{i}^{2}}{3Nk_{B}} \right) \] (1)

Fig. 1  MD simulation model for the nanometric machining of Cu/Ag bilayers.
碍于原子层的原子排列，材料在纳米尺度下会发生形变。因此，我们采用NVE（标准化）模型来模拟。MD快照通过上述方法展示。

在纳米成形和纳米刮擦阶段，温度的变化应被考虑。在纳米成形和纳米刮擦阶段，温度会略有增加。当温度变化大于10 K时，工作件在静置阶段达到平衡状态。

使用MD模拟纳米加工包括三个阶段：放松阶段，纳米成形阶段和纳米刮擦阶段。工作件在其平衡状态下，纳米形变和纳米刮擦阶段往往会因热效应影响工作件。当工作件的温度在纳米尺度下波动时，工作件在其平衡状态下达到平衡。

在纳米成形和纳米刮擦阶段，热量的产生主要来自加工区。特别是在纳米刮擦过程中，加工区的热效应显著，工作件在纳米刮擦过程中达到平衡。

### 3. 机械和摩擦学性能

图2a-d展示界面匹配位错在Cu/Ag界面的（001）面上形成的界面结构，不同Cu薄膜厚度的界面结构。结果表明，当Cu薄膜厚度大于3 nm时，界面结构是稳定的。

在纳米刮擦过程中，界面匹配位错在不同晶面（110）和（111）的Cu薄膜上形成。在当前研究中，Cu薄膜厚度为3 nm和（001）面被选取，以研究界面控制的纳米成形行为在Cu/Ag双层中的表现。
The Young’s modulus of material is a key indicator, to assess the mechanical properties. Based on the Hertz contact mechanism, Young’s modulus of the substrate (Cu/Ag bilayers and pure Cu film) is given as followed:

\[
E_2 = \frac{1 - v_2^2}{\left( \frac{4\sqrt{Rh^3}}{3F} - \frac{1 - v_1^2}{E_1} \right)}
\]

where \(E_2\) is Young’s modulus of the substrate, \(F\) is indentation force, and \(R\) and \(D\) are the indenter radius and indentation depth. \(v_1\) and \(v_2\) denote Poisson’s ratios of the spherical indenter and substrate. \(E_1\) is Young’s modulus of the spherical indenter which is far higher than that of the substrate. So, it is regarded as infinite in comparison with Young’s modulus of the substrate. Hence, eqn (3) is simplified as followed:

\[
E_2 = \frac{3F(1 - v_2^2)}{4\sqrt{Rh^3}}
\]

According to eqn (4) and Fig. 3a, Young’s modulus in Cu/Ag bilayers and pure Cu film is calculated as 105 GPa and 123 Gpa, which is consistent with the previous experiment results of 115 GPa and 129 GPa.19–41

The hardness measurement is important for the evaluation of mechanical properties of materials. According to the previous work,14 the hardness \(H\), sometimes referred to as the contact pressure, is calculated as followed:

\[
\begin{align*}
H &= \frac{F_{\text{max}}}{A_c} \\
A_c &= \pi d_c^2/4 \\
r^2 &= (d_c/2)^2 + (r - h_c)^2 \\
h_c &= h_{\text{max}} - \epsilon F_{\text{max}}/S
\end{align*}
\]

![Fig. 2](image-url)

The \(x\)–\(y\) sectional views of interface mismatch dislocations at different Cu film thicknesses: 1 nm (a), 2 nm (b), and 3 nm (c), and 10 nm (d) on the (001) plane. Interface mismatch dislocations at the Cu film thickness of 6 nm and different crystal planes: the (110) plane (e), and the (111) plane (f).
where $F_{\text{max}}$ is the maximum indentation load, and $A_c$ is the projected area of the indenter at the maximum indentation depth. $d_c$ is the diameter of the residual impression in the indented surface, $r$ is the indenter radius, and $h_c$ is used to calculate the projected contact area obtained by Sneddon’s equation. $h_{\text{max}}$ is the maximum indentation depth. Based on the general principles of elastic and elastic-plastic contact during indentation at the nanometre scale from ref. 44, the value of $\varepsilon$ is 0.75 for a spherical indenter. The contact stiffness of $S$ is obtained by fitting the unloading force–displacement curve. Because $S$ tends to $\infty$ in the unloading process, $h_c$ is close to $h_{\text{max}}$. The area $A_c$ can be calculated as followed:

$$A = \pi(2r - h_{\text{max}})h_{\text{max}}$$  \hspace{1cm} (6)

Hence, the hardness can be obtained by the equation:

$$H = \frac{F_{\text{max}}}{\pi(2r - h_{\text{max}})h_{\text{max}}}$$  \hspace{1cm} (7)

Based on eqn (7), the hardness of pure Cu film is calculated as 14.6 GPa, which is closed to the simulation value of 14 GPa and the experiment value of 12.4 GPa. The hardness of Cu/Ag bilayers is calculated as 10.3 GPa, and smaller than that of pure Cu film.

Fig. 3a shows the curves of indentation force versus the indentation depth. Here, the indentation force is defined as the force acting on the indenter along z-direction, which is measured by summing the forces of all the indenter atoms along z direction. The indentation forces firstly increase linearly, indicating the occurrence of the elastic deformation. After the elastic deformation, the indentation forces fluctuate owing to the dislocation movement. As a result, the plastic deformation occurs in Cu/Ag bilayers and pure Cu film.

Low Young’s modulus and hardness above mentioned are attributed to the interface-weakening effect. In order to reveal the interface-weakening effect in Cu/Ag bilayers, the x-z sectional views of Cu/Ag interface are shown in Fig. 3b and c. As the indenter penetrates into Cu/Ag bilayers during nano-indentation, a few dislocations propagate through the interface.
(I in Fig. 3b), and more dislocations are piled up at the interface. As a result, the mismatch dislocation network deforms, which inevitably leads to the severe local mismatch strain and stress concentrated in the core region of the mismatch dislocations, and lots of strain energy stored in the interface. Consequently, the new stacking faults in different slipping systems are activated from the Cu/Ag interface. The dislocations nucleate from the interface and emit into Cu film and Ag substrate to release the strain energy (II, III and IV in Fig. 3b and c), which makes the plastic deformation more easily in the Cu/Ag bilayers. Thus, the hardness of Cu/Ag bilayers is smaller than that of pure Cu film. In addition, the smaller hardness of Cu/Ag bilayers can also be understood from the electronic level. The electron density maps of atoms in the pure Cu film and Cu/Ag interface are plotted in Fig. 3d and e. The contours run from 0 to 1 electrons per Å³. It is seen from Fig. 3e that the electron density between Cu and Ag atoms is significantly smaller than that between Cu and Cu atoms in the Cu/Ag interface. Thus the bonding energy of Cu–Ag atoms is obviously weaker than that of Cu–Cu atoms in the Cu/Ag interface. Furthermore, the existence of Cu/Ag interface reduces the bonding energy of Cu–Cu atoms near the Cu/Ag interface (Fig. 3d and e). Hence the bond strength decreases due to the localization of the electron density, which is in good agreement with the previous work. The bond strength strongly influences, or even determines the hardness of solid. Thus the smaller hardness for Cu/Ag bilayers than pure Cu film can also be explained by the electron density and bond strength.

In order to reveal the effect of interface on the deformation of Cu/Ag bilayers during the nanometric machining, the changed interface energy is presented in Fig. 4a. With the tool advancing, the interface energy firstly increases and then tends to be stable, attributed to the effect of heat produced by machining. In addition, the interface energy fluctuates frequently during the nanometric machining, indicating the dislocation nucleation in the Cu/Ag interface at those points. Hence, the interface energy of Cu/Ag interface plays a significant role in the plastic deformation of Cu/Ag bilayers at the machining stage as well as the nanoindentation stage.

The tribological property of Cu/Ag bilayers can be expressed by the friction coefficient during nanometric machining process. In the current study, the friction coefficient is defined as the ratio of tangential force to normal force. According to the previous work, the surface energy plays a key role in the friction coefficient. Fig. 4b shows the average friction coefficient on the surfaces of (001) and (111) in pure Cu film during the stable machining stage. The friction coefficient on (001) surface is larger than that on (111) surface, attributed to that the surface energy of 2.166 J m⁻² on surface (001) is larger than that of 1.952 J m⁻² on surface (111) in pure Cu. The increase in surface energy could lead to an increase in the adhesion force. Hence, the friction coefficient decreases if Cu (111) surface instead of Cu (001) surface. In addition, for Cu/Ag bilayers, the average friction coefficient on (001) surface is also higher compared to the (111) surface. Moreover, the Cu/Ag bilayers have high friction coefficient, owing to the interface softening effect to increase the adhesion force.

4. Effect of machining parameters

The machining parameters, including tool radius, machining speed, machining direction and machining depth, would influence the subsurface damage and material removal during nanometric machining of Cu/Ag bilayers. Here, the average machining temperature, machining force and defect are carefully analyzed, to gain a good ground surface and low subsurface damage. In order to clearly understand the current study, the schematic illustration for the nanometric machining is shown in Fig. 5.

4.1. Effect of tool radius

Fig. 6a shows the variation curves of the average temperature during nanoindentation of Cu/Ag bilayers with different tool radii. The temperature rises as the indenter penetrates, and a larger indenter radius results in a higher temperature. This is because more severe extrusion occurs between atoms due to larger indentation depth or larger indenter radius. The extrusion would lead to the deformation of crystal lattices, and the strain energy is stored in deformation zone. Later the energy is released and transformed to heat when reaches the critical value. Thus, more thermal energy is produced by larger indenter radius. Fig. 6b reveals that the larger indentation force is
required under larger indenter radius. Namely, a larger tool–workpiece interaction zone is formed by a larger indenter radius. Therefore, more chippings are produced and larger indentation force is necessary to maintain the tool penetration with the certain speed.

The variation curves of the average temperature during nanometric machining with different tool radii of 3 nm, 4 nm and 5 nm are shown in Fig. 6c. Due to the effect of indenter radius on the temperature during nanoindentation process (Fig. 6a), there is a higher initial temperature in case of a larger indenter radius for the nanoscratching. The Cu/Ag bilayers have

![Diagram](image)

**Fig. 5** The schematic illustration for the nanometric machining of Cu/Ag bilayers.

![Graphs](image)

**Fig. 6** The average temperature (a) and indentation force (b) versus indentation depth. The average temperature (c) and machining force (d) versus machining distance during the nanometric machining of Cu/Ag bilayers with different tool radii of 3, 4 and 5 nm.
a good thermal conductivity, thus the heat from the machined region can be transferred to thermostat atoms during nanoscratching process. However, Fig. 6c shows that the average temperature keeps rising and then steady as the tool advances. This is because the temperature little diffuses from the machined region to the thermostat atoms at beginning of the scratching stage, and then the heat dissipation rate sharply increases with the increment of the machining distance, until the balance between heat dissipation rate and the heat production rate.\(^{26}\) Thereby the average temperature is finally stabilized at a constant. In addition, the temperature increases with the increment of indenter radius. The smaller indenter radius produces less thermal energy and makes temperature of workpiece balanced more quickly. With the increment of machining distance, the machining force first increases rapidly because of the increased atom number around the indenter, and then fluctuates nearby the corresponding constant values, as shown in Fig. 6d. The fluctuation is due to the occurrence of dislocation events during nanometric machining process. The glide of dislocations successively emitted from the tool–workpiece interaction zone leads to the increment of machining force. The dislocations passed through Cu/Ag interface, and the dislocations nucleated and emitted from the interface release the strain energy and cause the decrease of machining force. In addition, as the larger indenter radius induces more lattice defects in the machining zone, thus Cu/Ag bilayers are strengthened and larger machining force is required to maintain indenter advancing at a constant speed.

In addition, the friction coefficients of Cu/Ag bilayers and pure Cu film fluctuate with the increasing machining distance, attributed to the normal vibration of crystal lattice and the work-hardening during the nanometric machining process.\(^{30}\)

The \(y-z\) plane cross-section snapshot of Cu/Ag bilayers for three different tool radii is shown in Fig. 7a–c, and the top view of surface morphology is presented in Fig. 7d–f. As the tool advances, the primary shear stress would be larger than the critical shear stress required for dislocation nucleation and slipping, which releases the strain energy in Cu/Ag bilayers. Fig. 7a–c indicates that the atomic lattice distortion becomes severer under the larger indenter radius. In addition, the thermal activation induced larger indenter radius also promotes the formation of defects. Thus the number of ISF atoms increases and more dislocations nucleate in case of larger indenter radius. Fig. 7d–f shows the surface morphology of Cu/Ag bilayers with different indenter radii. There is less volume of the chipping around the ground surface at smaller indenter radius. As the machining distance increases, more atoms are accumulated. Later the atoms emerge on the surface and grow into chipping. The chipping formation is a atomic extrusion process,\(^{52-54}\) during which dislocations nucleate, glide on the \(\{111\}\) slip planes and lastly terminate at the workpiece surface.\(^{9,55}\) Base above discussions, the smaller indenter radius

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Fig. 7 The instantaneous structure (a–c) and surface morphology (d–f) of the deformed Cu/Ag bilayers at different tool radii of (a and d) 3 nm, (b and e) 4 nm and (c and f) 5 nm.
should be selected to reduce the subsurface damage during the nanometric machining process of Cu/Ag bilayers.

4.2. Effect of tool speed

According to the previous work, a general machining speed is less than 45 m s\(^{-1}\), a high machining speed of 45–150 m s\(^{-1}\), and a ultra-high machining speed is more than 150 m s\(^{-1}\). In order to investigate the effect of tool speed on the nanometric machining of Cu/Ag bilayers, three speeds of 20, 100, 200 m s\(^{-1}\) are selected in the simulations.

Fig. 8a shows the evolution of the average temperature during the indenter penetrating into the Cu/Ag bilayers. It is found the temperature is affected slightly by the tool speed during nanoindentation process. The variation of indentation force versus indentation depth at different tool speeds is shown in Fig. 8b. As the lattice defects do not have sufficient time to recover or adjust and new lattice defects continue to form under the high-velocity nanoindentation, the Cu/Ag bilayers are strengthened. Therefore, the larger indentation force is needed for the indenter penetration and further plastic deformation at higher velocity. When the indentation depth is reached 1.5 nm, the nanoscratching is conducted. Fig. 8c shows the increased number of different types of atoms at machining speed of 100 m s\(^{-1}\). It is seen that the FCC atomic number decreases with the increment of ISF and other atoms (zone I and III), indicating that plastic deformation of Cu/Ag bilayers is dominated by the dislocation nucleation and propagation. In addition, zone II shows the different types of atom number fluctuate slightly, which can be ascribed to the interaction of dislocations. The

![Fig. 8](image-url)
dislocation intersection would restrict the dislocation motion, and lead to the hardening and lower plasticity. And some dislocations can be absorbed by mismatch dislocations of interface.\textsuperscript{17} Fig. 8d shows the evolution of different types of atom number versus machining distance during nano-scratching with different tool speeds. Due to the less time for the rearrangement of deformed atom lattices at high-velocity machining, more dislocation cores appear in Cu/Ag bilayers. Thus the number of ISF atoms displays little variation, but that of other atoms increases with the increment of tool speed.

Fig. 8e shows the evolution of the average temperature versus machining distances at different machining speeds. Under a higher machining speed, the friction between atoms is more drastic. Consequently more friction energy is released from the deformed crystal lattices and further transformed to the machining heat. The machining heat would diffuse toward the thermostat layer. Since the tool needs the less time to complete the same machining distance at a higher machining speed, thus the less time is provided to heat diffusion, which causes higher temperature for Cu/Ag bilayers in case of higher machining speed. In addition, due to the increment of heat dissipation rate as the tool advances, until the balance between heat dissipation rate and the heat production rate,\textsuperscript{26} the temperatures finally become steady, as shown in Fig. 8e.

Fig. 8f shows the average machining forces at different machining speeds, and the error bar represents the average error between the machining forces and the average machining force during stable machining process of Cu/Ag bilayers. The average machining force is larger at the higher machining speed, which involves with the dislocation generation events during the material removal process.\textsuperscript{56} Due to the lower machining speed than the propagation speed of a plastic wave, the dislocations propagate away from the tool–workpiece interaction region more easily and more dislocations nucleate under higher machining speed (Fig. 8d). This strengthens the Cu/Ag bilayers and larger machining force is needed for the high-speed advancement of tool.\textsuperscript{26}

Fig. 9a–c display the surface morphology of Cu/Ag bilayers at different machining speed. In order to exhibit the chipping volume, the atoms are colored depending on atomic height. It is seen that machining speed has a significant influence on the volume of the chipping pileup. A comparison of Fig. 9a–c demonstrates that a larger volume of chippings appear under a higher machining speed. In addition, the quality of ground surface varies with the machining speed. The effect of machining speed on groove roughness is certified in Fig. 9d. The groove roughness is named as $R_{\text{max}}$ which is the maximum height asperity of the groove area along the machining direction, and is the average distance between the highest point within the asperity and the lowest point within the groove.\textsuperscript{57} Fig. 9d describes that the increasing machining speed generates the increment of groove roughness, and the variation of the groove roughness to machining speed is more sensitive at a low speed. Based on above discussions, the selection of a low machining speed is beneficial to reduce the subsurface damage and improve the smoothness of ground surface during nanometric machining of Cu/Ag bilayers.

4.3. Effect of machining depth
The machining depth $h_{\text{max}}$ is maximum indentation depth achieved during the nanoindentation process, and the tool cuts...
workpiece at this depth in the nanometric machining process. Fig. 10 shows the instantaneous deformed structure and surface morphology of Cu/Ag bilayers at different machining depths of 1, 1.5 and 2.5 nm. Fig. 10a–c are the corresponding snapshot in x–y cross-section, where atoms are colored according to the CNA values. It can be seen from Fig. 10d–f the chipping volume at different machining depths, where atoms are colored according to atomic height. Under larger machining depth, more lattice defects are observed in machining zone (Fig. 10a–c). Correspondingly, more chippings are generated around the groove (Fig. 10d–f). When the machining depth is relatively larger, more atoms around the tool are extruded and emerge on the surface later, thereby more chippings pile up on the surface. Due to the existence of external stress field beneath the tool, the
arrangement of Cu atoms in the tool–workpiece interaction zone sharply changes. As a result, the nucleation and slipping of partial dislocation along $\{111\}$ slip planes dominate the plastic deformation of Cu/Ag bilayers during nanometric machining.

Fig. 11a describes the variation of machining force versus machining distances at different machining depths of 1, 1.5 and 2.5 nm. Since more lattice defects are induced by larger machining depth in the machining zone (Fig. 10a–c), the Cu/Ag bilayers is strengthened more severely and a larger machining force is required to keep cutting at the constant speed of 100 m s$^{-1}$. The evolution of the average temperature versus machining distance is shown in Fig. 11b. There is higher initial temperature under larger machining depth for the nano-scratching of Cu/Ag bilayer, which is attribute to the effect of nanoindentation process. Namely, the larger indentation depth would inevitably cause the higher temperature during nanoindentation. In the following nanoscratching process, the average temperature evolution follows a similar rule with machining forces. The larger machining depth leads to higher temperature. Therefore, the smaller machining depth could reduce subsurface damage by relatively less ISF atoms, and decrease energy consumption by relatively low temperature.

5. Conclusions

Three dimensional MD simulations of nanometric machining process on Cu/Ag bilayers and pure Cu film are conducted to study the mechanical and tribological properties of Cu/Ag bilayers. The effects of machining parameters on the subsurface damage and material removal of Cu/Ag bilayers are also investigated by changing the indenter radius, tool speed and machining depth during nanometric machining. Based on the above discussions, conclusions can be drawn as follows:

(1) Due to the dislocation nucleation and emission from the Cu/Ag interface, the hardness of Cu/Ag bilayers is smaller than that of pure Cu film. The Cu/Ag bilayers have a larger friction coefficient than pure Cu film. In addition, the metal bonding energy in Cu/Ag interface is weaker than that in pure Cu film, which also induces the hardness of Cu/Ag bilayers to be smaller than that of pure Cu film. Young’s modulus in Cu/Ag bilayers and pure Cu film is calculated by the Hertz contact mechanism and close to experiment result.

(2) Comparing different indenter radii, the chipping volume and the number of ISF atoms beneath the indenter increase with the increment of the indenter radius during nanometric machining of Cu/Ag bilayers. The larger indenter radius causes larger heat dissipation, thereby more defects are induced by thermal activation. Thus, a smaller indenter radius should be selected for the nanometric machining to reduce subsurface damage via relatively less ISF atoms and lower machining heat.

(3) The selection of lower tool speed is crucial to reduce the subsurface damage and improve the smoothness of ground surface. The higher tool speed would produce more chippings and larger groove roughness. Simultaneously, the high-speed machining needs to be maintained by the larger machining force. The higher temperature is caused by the higher tool speed and further induces more defects.

(4) With decrease of machining depth, the chipping volume and the number of defect atoms reduce sharply, resulting in the decreasing of subsurface damage at the smaller machining depth.

Conflicts of interest

There are no conflicts to declare.

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References

1. Z. Zhang and H. M. Urbassek, J. Mater. Sci., 2018, 53, 799.
2. T. Fu, X. Peng, X. Chen, S. Weng, N. Hu, Q. Li and Z. Wang, Sci. Rep., 2016, 6, 35665.
3. Q. H. Fang, Q. Wang, J. Li, X. Zeng and Y. W. Liu, RSC Adv., 2017, 7, 42047.
4. L. F. Zeng, R. Gao, Q. F. Fang, X. P. Wang, Z. M. Xie, S. Miao and T. Zhang, Acta Mater., 2016, 110, 341.
5. C. Zhang, K. Feng, Z. Li, F. Lu, J. Huang and Y. Wu, Appl. Surf. Sci., 2016, 378, 408.
6. C. Wang, J. M. Pureza, Y. Yang and Y. W. Chung, Surf. Coat. Technol., 2016, 288, 179.
7. B. Wang, Z. Zhang, K. Chang, J. Cui, A. Rosenkranz, J. Yu and N. Jiang, Nano Lett., 2018, 18, 4611.
8. A. Reserbat-Plantey, K. G. Schädler, L. Gaudreau, G. Navickaite, J. Güttinger, D. Chang and F. H. Koppens, Nat. Commun., 2016, 7, 10218.
9. J. J. Zhang, C. Begau, L. Geng and A. Hartmaier, Wear, 2015, 332, 941.
10. S. Goel, X. Luo, A. Agrawal and R. L. Reuben, Diamond machining of silicon: a review of advances in molecular dynamics simulation, Int. J. Mach. Tools Manuf., 2015, 88, 131–164.
11. L. Midolo, A. Schliesser and A. Fiore, Nat. Nanotechnol., 2018, 13, 11.
12. Z. Zhang, B. Wang, S. Huang, B. Wen, S. Yang, B. Zhang and D. Guo, Mater. Des., 2016, 106, 313.
13. D. D. Cui and L. C. Zhang, Adv. Manuf., 2017, 5, 20.
14. J. J. Zhang, Z. F. Wang, T. Sun and Y. D. Yan, Mater. Res. Express, 2016, 3, 125018.
15. B. Wang, Z. Zhang, J. Cui, N. Jiang, L. Lyu, G. Chen and F. Ye, ACS Appl. Mater. Interfaces, 2017, 9, 29451.
16. J. Li, Q. H. Fang, B. Liu and Y. W. Liu, Acta Mater., 2018, 147, 35.
17. C. Begau, A. Hartmaier, E. P. George and G. M. Pharr, Acta Mater., 2011, 59, 934.
18. H. Hertz, J. Reine Angew. Math., 1882, 92, 156.
19 S. Shao and S. N. Medyanik, Mech. Res. Commun., 2010, 37, 315.
20 T. H. Fang and J. H. Wu, Comput. Mater. Sci., 2008, 43, 785.
21 D. Cheng, Z. J. Yan and L. Yan, Thin Solid Films, 2007, 515, 3696.
22 J. McKeown, A. Misra, H. Kung, R. G. Hoagland and M. Nastasi, Scr. Mater., 2002, 46, 593.
23 J. B. Liu, L. Zhang, D. W. Yao and L. Meng, Acta Mater., 2011, 59, 1191.
24 C. Zhao, X. Zuo, E. Wang, R. Niu and K. Han, Mater. Sci. Eng., A, 2016, 652, 296.
25 Y. Y. Tian, J. Li, Z. Y. Hu, Z. P. Wang and Q. H. Fang, Chin. Phys., 2017, 26, 162802.
26 J. Li, Q. H. Fang, Y. W. Liu and L. C. Zhang, Appl. Surf. Sci., 2014, 303, 331.
27 J. Stadler, R. Mikulla and H. R. Trebin, Int. J. Mod. Phys. C, 1997, 8, 1131.
28 A. Stukowski, Modell. Simul. Mater. Sci. Eng., 2010, 18, 015012.
29 J. D. Honeycutt and H. C. Andersen, J. Phys. Chem., 1987, 91, 4950.
30 T. Fu, X. H. Peng, Y. Zhao, B. C. Feng, C. Huang, Q. B. Li and Z. H. Wang, Appl. Phys. A, 2016, 122, 67.
31 Y. Q. Geng, J. J. Zhang, Y. D. Yan, B. W. Yu, L. Geng and T. Sun, PLoS One, 2015, 10, 0131886.
32 S. Goel, X. Luo, A. Agrawal and R. L. Reuben, Int. J. Mach. Tools Manuf., 2015, 88, 131–164.
33 Z. F. Wang, J. J. Zhang, H. ul Hassan, J. G. Zhang, Y. D. Yan, A. Hartmaier and T. Sun, Int. J. Mech. Sci., 2018, 148, 531–539.
34 J. Li, Q. H. Fang, B. Liu, Y. W. Liu and Y. Liu, RSC Adv., 2016, 6, 76409.
35 P. Peng, G. L. Liao, T. L. Shi, Z. R. Tang and Y. Gao, Appl. Surf. Sci., 2010, 256, 6284.
36 S. M. Foiles, M. I. Baskes and M. S. Daw, Phys. Rev. B, 1986, 33, 7983.
37 M. S. Daw, S. M. Foiles and M. I. Baskes, Mater. Sci. Rep., 1993, 9, 251.
38 H. Gercek, Int. J. Rock Mech. Min. Sci., 2007, 44, 1.
39 M. Verdier, H. Huang, F. Spaepen, J. D. Embury and H. Kung, Philos. Mag., 2006, 86, 5009–5016.
40 S. I. Hong and M. A. Hill, Acta Mater., 1998, 46, 4111.
41 T. D. Shen, C. C. Koch, T. Y. Tsui and G. M. Pharr, J. Mater. Res., 1995, 10, 2892.
42 H. Zhao, C. Shi, P. Zhang, L. Zhang, H. Huang and J. Yan, Appl. Surf. Sci., 2012, 259, 66.
43 I. N. Sneddon, Int. J. Eng. Sci., 1965, 3, 47.
44 A. C. Fischer-Cripps, Nanoindentation, New York, 2004, pp. 1–20.
45 C. Qiu, P. Zhu, F. Fang, D. Yuan and X. Shen, Appl. Surf. Sci., 2014, 305, 101.
46 D. Saraev and R. E. Miller, Acta Mater., 2006, 54, 33.
47 D. Beegan, S. Chowdhury and M. T. Lauzier, Surf. Coat. Technol., 2005, 192, 57.
48 G. V. Gibbs, D. F. Cox and K. M. Rosso, J. Phys. Chem. A, 2004, 108, 7643.
49 D. J. González, L. E. González and M. J. Stott, Phys. Rev. Lett., 2004, 92, 085501.
50 W. R. Chang, I. Etsion and D. B. Bogy, J. Tribol., 1988, 110, 57.
51 L. Vitos, A. V. Ruban, H. L. Skriver and J. Kollar, Surf. Sci., 1998, 411, 186.
52 J. Li, Q. H. Fang, B. Liu and Y. W. Liu, Appl. Surf. Sci., 2016, 384, 419.
53 J. Li, Q. H. Fang, Y. W. Liu and L. C. Zhang, Int. J. Adv. Des. Manuf. Technol., 2015, 77, 1057.
54 X. Zhu, H. Hou, X. Huang, M. Zhou and W. Wang, Constr. Build. Mater., 2012, 29, 476.
55 G. Ziegenhain, H. M. Urbassek and A. Hartmaier, J. Appl. Phys., 2010, 107, 061807.
56 Y. Liu, B. Z. Li and L. F. Kong, Comput. Mater. Sci., 2018, 148, 76.
57 F. Sun, S. Qu, Y. Pan, X. Li and C. Yang, Int. J. Adv. Des. Manuf. Technol., 2014, 73, 613.