Nanoindentation and Deformation of Multilayered Au/Cu Films

Yu-Cheng Fan, Te-Hua Fang, Kuan-Ming Lin and Ren-Zheng Qiu
Department of Mechanical Engineering, National Kaohsiung University of Applied Sciences, Kaohsiung, Taiwan

ABSTRACT
The mechanical properties of single and multilayer gold and copper films are studied using molecular dynamics and deformation, the slip effect, the load bearing capacity and energy differences are also discussed. Results showed that as the indentation depth increases in a multilayer model, the grain boundaries of the first layer are broken and the atoms diffuse into the lower layer, thereby leading the change of the amount of slip. Single-crystal Au and Cu models generate more slippage due to lower bond energy between atoms. The larger the amount of atomic flow under indentation is, the larger the amount of slip is. As the depth of the indentation increases, the area influenced by indentation increases and the maximum load bearing capacity and potential energy also increase. Plastic deformation from indentation at high speed does not result from dislocation slip, but from a larger force that destroys the bonds between atoms. At higher temperature, the amount of slip around the indenter is less obvious and the structure is gradually softened. Moreover, the same depth of indentation can be achieved with a smaller load force for higher temperature.

1. Introduction
Both the scanning probe and atomic force microscope are useful tools for a study of the surface and the mechanics of thin films by the use of the nanoindentation technique [1–3]. The development of nanotechnology is almost dependent on breakthroughs made in the laboratories of materials processing manufacturers [4,5]. The search for smaller, lighter, and thinner precision materials is
Continuous [6]. Progress in multilayer film technology can promote development in many other industries, and thin films are widely used in the photovoltaic industry and machinery industry which are deeply invested in related research [7]. Even the textile industry has developed nanoscale fabrics, which have both sterilization and deodorization function. At present, research is predominantly concentrated on multilayer nanofilms. The grain refinement strengthening effect of nanomultilayer film grain boundary is excellent. Moreover, the overall area is very large. High strength and excellent abrasion resistance are important nanomultilayer film properties [8,9]. Image of its high-resolution sample of nanostructures may be observed by a scanning electron microscope [10], and it contributes to the design and manufacture of nanostructures.

Simulation studies of the molecular dynamics of materials have provided very useful nanomechanical results [11]. In this study, molecular dynamics has been used to simulate the nanoindentation of gold–copper–gold nanomultilayer films. Indenters of different shapes at different temperature expose the properties of both the material and the actual technology. The relationship between energy change and load carrying capacity at different temperatures as well as the amount of atomic slip at different indentation speed and depth of the substrate are explored. A major trend in technological development today is towards miniaturization at a nanolevel. Materials at a nanoscale often exhibit many different, sometimes unexpected, physical properties. Moreover, the demand for high quality precision machining is going up steadily. Properties such as hardness after molding with different force and speed, deformation of the mold itself and many other related effects and problems are important.

The purpose of this study was to carry out simulation experiments on multi-layers by nanoindentation and to use molecular dynamics to examine the results. Mechanical properties relating to different layers and alloys are also discussed. It is abundantly clear that nanometer manufacturing processes can be improved and the future of nanotechnology applications can be enhanced.

2. Molecular Dynamics

A basic model was first established for the simulation of nanoindentation, where the indenter was a trapezoidal pyramid consisting of 8580 carbon atoms. A diamond structure was chosen for the indenter because it could be defined as a rigid body without wear. The substrate was a face-centered cubic crystal stacked in three alternating layers of gold and copper atoms 4.15 nm (X) × 12.45 nm (Y) × 6.46 nm (Z). Figure 1 is a schematic diagram of the multi-layer atomic model and the indenter. The indenter and the substrate were set as rigid bodies. Two layers of atoms at the bottom of the substrate are set as fixed throughout the simulation. The remainder was defined as an atomic moving layer and periodic boundary conditions were given. The system temperature in the initial heat balance process was set to 300 K. The indenter atoms were defined as a rigid body immune to deformation irrespective of temperature or load changes.

In terms of periodic boundary conditions, the X-axis and Y-axis directions were set and the Z-axis was true height without boundary conditions. After the model has been constructed, the indenter was given a set speed parameter. Initially indentation simulation was carried out on the XY plane of the substrate along the −Z axis at a steady rate. The values and characteristics of the interactive relationship between the slip state and the various mechanisms were then obtained.

In this study, the gold and copper atoms are solid metal. To select the potential energy function, we used the tight-binding multi-body potential, to simulate interaction between the forces inside the substrate. The Morse potential [12] was used to calculate potential energy between the indenter and the substrate:

$$\Phi(r_{ij}) = D \cdot \left\{ e^{-2\alpha (r_{ij} - r_0)} - 2 \cdot e^{-\alpha (r_{ij} - r_0)} \right\}$$ (1)

In Equation (1) $\alpha$ is an elastic coefficient parameter of the material, $D$ is binding energy, and $r_0$ is the balanced distance between atoms obtained by the spectral data.

The tight-binding potential function is generally used to describe the effect of the noble metal atoms represented in Equation (2), where $E_{rep}$ is the repulsion energy (eV), $E_{bond}$ is the bond term (eV), represented by Equation (3) and (4) [13].

Figure 1. Schematic diagram of a multilayer nanofilm.


\[ E_c = \sum_i (E_B^i + E_R^i) \]  

(2)

\[ E_B^i = -\left\{ \sum_{j \neq i} \xi^2 e^{-2q\left(\frac{r_{ij}}{\xi} - 1\right)} \right\} \]  

(3)

\[ E_R^i = \sum_j A e^{-p\left(\frac{r_{ij}}{\xi} - 1\right)} \]  

(4)

3. Results and Discussion

We used the same trapezoidal indenter at a system temperature of 300 K, and its associated parameter conditions were fixed. The indenter velocity used was 100 m/s, and the simulated indentation was to a depth of 2.0 nm from an initial depth of 0 nm, as shown in Figure 2. In the process, when the indenter is about to touch the substrate surface, an interactive force is generated between the indenter and the substrate, which leads to the vibration of surface atoms. The substrate is squeezed by the indenter as it continues to move downwards and the atomic structure undergoes changes. The atoms on both sides of the indentation begin to move towards free space and both sides of the substrate bulge upwards. As the indenter continues to move downwards, the original substrate structure that underwent elastic deformation, now undergoes plastic deformation that continues until the indenter stops applying force.

3.1. The Deformation Mechanism in Au and Cu Single Crystal and Multilayer Models

Simulated indentation was done using a sufficient force to cause penetration of the indenter to depths of 1 and 2 nm from an initial depth of 0 nm, as shown in Figure 2. In the process, when the indenter is about to touch the substrate surface, an interactive force is generated between the indenter and the substrate, which leads to the vibration of surface atoms. The substrate is squeezed by the indenter as it continues to move downwards and the atomic structure undergoes changes. The atoms on both sides of the indentation begin to move towards free space and both sides of the substrate bulge upwards. As the indenter continues to move downwards, the original substrate structure that underwent elastic deformation, now undergoes plastic deformation that continues until the indenter stops applying force.

3.1.1. Slip Structure Analysis

In this section, the slip state diagrams of the different materials and layers are discussed. In Figure 2, it can be seen that the largest amount of slip occurs in the region where the indenter makes contact with the substrate. The indenter load bearing capacity, as well as the periodic boundary effect and blocking by grain boundary energy, causes the atoms to push against each other, thereby leading to the plastic deformation of the structure.
The distribution of the amount of slip exhibited by each type of substrate is uneven. Au and Cu show more slips than the layered substrate because their interatomic bonding energy is lower and the atomic flow under pressure is higher.

It was found that no obvious dislocations within the substrate occur for Au and Cu at an indentation depth of 0.1 nm. At an indentation depth of 1 nm, both sides close to the periodic boundary generate a significant amount of slippage. The reasons for this are presumed to be the lower atomic bonding force in the substrate and the fact that the atoms are influenced by the tapered shape of the indenter which can easily move them aside. Another reason is the composition ratio of the material which has lower interatomic stability. Under load the outer layer of atoms expands easily and more slip occurs. When the indentation depth reaches 2 nm, the indenter has already come to rest. There is a large amount of displacement in the area between the indenter and the substrate where a slip plane has formed.

At an indentation depth of 1 nm, in the multilayer nanofilm model, the load on the substrate at the indenter substrate contact surface causes a large amount of dislocation. However, the grain boundary between the layers is strong and resists displacement. The slip region stays at the top of the first layer, obstructed by the grain boundary, and does not move to the layer below. It is more specifically observed that there is intensive plastic deformation in the area above the atomic grain boundary of the upper layer. This barrier causes the atoms to move sideways but not downwards and they do not penetrate to the lower layer of atoms. As a result, the atoms below diffuse and slide in irregular directions. When the indenter goes downwards far enough to touch a grain boundary, the boundary is extruded and the force exerted by the indenter disrupts the boundary which no longer acts as a block to dislocation and gradually disappears. Therefore, the atoms of the top layer are now able to move through the crystal boundary and diffuse into the structure of the lower layer. The atoms are densely stacked and squeezed to produce slip bands. The slip bands arise as a result of intense force from the indenter which generates dislocations. When a dislocation moves along a specific crystal boundary, a slip plane is formed on the boundary.

When the indentation depth reaches 2 nm, the multi-grain boundaries in the model impede downwards atomic displacement and dislocation only arises at the grain boundaries. When the force exerted by the indenter gets close to the grain boundary layer, the upper layer atoms begin to move downwards towards the lower layer structure and diffuse sideways into the substrate to form dislocations, thereby leading the occurrence of the nucleation and the growth phenomenon.

### 3.1.2. Temperature Effect Analysis

This section focuses on the influence of temperature arising post-indentation in the simulation of different single crystal and multilayer alloy models. At an indentation depth of 1 nm in a monocrystalline Au substrate (see Figure 4), the ductility of gold allows the deformation to take the form of a bulge around the indenter. During structural deformation, more strain can produce dislocations and the temperature around the indenter is also significantly higher than in the other models.

For simulations at 2-nm indentation depth (for all the models), the temperature in the area of contact between the substrate and indenter show a significant rise. With the subsequent increase in atomic kinetic energy, atomic activity also increases and interaction becomes easier. The material become softer and the atomic slip vector value will rise [14].
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stability, which is especially evident in the single-crystal Cu substrate. The atoms undergo severe shock causing outwards diffusion, and the energy curve shows a significant rise. When the indentation process reaches around 25 ps, the substrate energy rises steeply. Here, energy is enhanced by intense activity between atoms under elastic deformation. When the elastic limit has been passed, the material undergoes plastic deformation and the speed energy curve continues to rise (as penetration continues) until indentation stops.

3.1.3. Load-bearing Capacity Analysis

Since the depth of the indentation is proportional to the time of the indentation, the displacement of the indentation is represented by the time in this article. The force−displacement curves for the different substrates in Figure 5 show that before indentation the value is close to zero. There is no interaction because the indenter has not yet entered the cut-off radius of the substrate atoms. As indentation force increases and penetration reaches 1 nm into the substrate, the force−displacement curve first falls a little and then rises to show that interatomic forces have begun to take effect. The drop is caused by a jump state when the atmospheric pressure drops around the indentation before the repulsive force from the indenter takes effect and the curve begins to rise. It can be seen from the figure that the indenter forces for single-crystal Au and Cu, and the three and five layer models are not the same. The maximum loads are 1100, 700, 1000, and 900 nN, respectively, for the four models.

Because the different substrate materials have different thermal equilibrium, atomic crystal lattice energy and structure composition, the initial energy is different, see Figure 6. It can be seen that near the displacement time of 10 ps, when the indenter makes contact with the substrate, the energy curve for each type of substrate begins to rise. This energy fluctuation shows that the substrate is unstable, which means that the crystal structure affects the release of energy [15]. The energy level is related to atomic

Figure 4. Single-crystal Au and Cu and multi-layer model temperature state.

Figure 5. Single-crystal Au and Cu and strength displacement of the multilayer model.
it reaches a depth of 2 nm. It can be seen that when the extruded deformation area of the substrate increases and spreads out, the extruded deformation area of the 6-nm wide rectangular indenter is significantly larger than that of the trapezoidal one. This is because the greater the force-sustaining contact area between indenter and the substrate, the greater the number of mobile atoms. Affected areas are concentrated around the area of contact between the second layer of the substrate and the indenter. After the diffused atoms fail to disrupt the grain boundary, they move down to the lower layer. Therefore, the atoms do not yet enter the bottom layer.

3.2.2. Slip Structure Analysis
The differences between the slip states resulting from indentation by three different indenters is discussed in this section. Sectional views of substrates indented to 1 and 2 nm by indenters of different shape and size are shown in Figure 8. In the figure, it can be seen that the trapezoidal indenter with a small contact area, shows a smaller and slower amount of atomic displacement. With the increased depth of indentation and the barrier of a grain boundary, causes the atoms to accumulate near the surface of the substrate around the indentation and they also diffuse outwards. The indents of different size and shape generate different degrees of dislocation. This is particularly

3.2. The Types of Indenter Used in the Simulations
The associated parameters were fixed as: system temperature of 300 K, indentation velocity of 100 m/s, and the final indentation depth 2 nm. The Au–Cu–Au multilayer nanofilm was chosen as the substrate model to be used for exploration of the changes in slip and mechanical properties of the different indenters used in the simulations.

3.2.1. Multilayer Model Deformation Mechanism for Different Types of Indenter
The 4 nm × 6 nm indenter shown in Figure 7 has a trapezoidal shape. The chamfered edges of the indenter change the direction of interatomic interaction as it moves into the substrate to a final depth of 1 nm. This causes the atoms extruded by penetration to move in different directions as penetration proceeds. The atoms were subject to a downwards load and pushing pressure was generated, which disrupted the grain boundary layer. Then, atoms diffused past the boundary layer towards the lower layers where they aggregated.

The initial model is set to a fixed layer in cycle boundary and the bottom. Therefore, the indenter downwards force was affected by the cycle boundary. The sphere of influence is confined to the area around the indenter in contact with the second layer, and indenter stops when it reaches a depth of 2 nm. It can be seen that when the extruded deformation area of the substrate increases and spreads out, the extruded deformation area of the 6-nm wide rectangular indenter is significantly larger than that of the trapezoidal one. This is because the greater the force-sustaining contact area between indenter and the substrate, the greater the number of mobile atoms. Affected areas are concentrated around the area of contact between the second layer of the substrate and the indenter. After the diffused atoms fail to disrupt the grain boundary, they move down to the lower layer. Therefore, the atoms do not yet enter the bottom layer.

Figure 6. Monocrystalline Au and Cu and multi-layer model energy.
in the amount of slip plane surrounding the indenter, the amount of slip inside the substrate also begins to focus, where the number of slip atoms is greatest for the 4 and 6 nm wide indenters. It can be seen that the material properties affect the slip state of the substrate atoms, and there is a direct correlation between slip state and the area of the indenter in contact with the substrate [16].

Figure 7. Various types of indenter model indentation schematic state diagram.

Figure 8. Various types of indenter model slip state diagram.
3.2.3. Load-bearing Capacity Analysis
When the indenter approaches the substrate in these simulations, the indenter load and downwards speed are close to zero and the difference is insignificant, as shown in Figure 9. The maximum load capacities of different indenters Type 1, Type 2, Type 3 are 1100, 1200, and 2000 nN, respectively. When the indenter starts to come into contact with the substrate atoms, they begin intense vibration. The force also begins to increase. Since the contact areas between the indenter and the substrate are different, loading capacity appears different and the force curve of a Type 3 indenter is significantly higher. As the indenter goes deeper, the force continues to rise. A micro amplitude band arises mainly from the energy boost from the intense activity between the material atoms as it is squeezed. However, when plastic deformation begins, a slight decrease of the force curve is seen. After this, the indenter force curve continues to rise until indentation stops.

The energy changes generated between indenters with different contact areas and shapes and the different substrates was studied. It was found that just before contact was made between the indenter and the substrate surface, the initial energy gap for the different indenters varied by about 4%. This difference is due to the different number of atoms in the various indenters. In this initial stage, the atoms are in a state of shock and the energy band is unstable. After the indenter contacts the substrate, the state of atomic shock subsides and the band becomes steady. With an increase in downwards pressure on the area of contact between the indenter and the substrate, the substrate atomic spacing is pushed. Kinetic energy, which diffuses outwards is produced, and atomic structural deformation takes shape. When indentation stops, strong adsorption energy is formed. This further disrupts the structure and may increase the stress value and energy. The different shapes of indenters and the substrate squeeze angles lead to different flow between affected atoms. Because the areas of contact between the indenter and the substrate are different, the amount of atomic adsorption is different. The energy values also changed.

3.3. The Different Rates of Nanoindentation
To investigate the effect of indentation speed on the atomic structure of the substrate, simulated indentations to 2 nm were carried out at 50, 100, and 200 m/s at an initial temperature of 300 K. Impact on the substrate by the indenter at different indentation speeds is discussed.

3.3.1. The Multilayer Deformation Mechanism for Various Types of Indenters
When the indenter approaches the substrate, the surface atoms of the substrate are attracted to those of the indenter. This continues until the indenter contacts the substrate and compression starts. The substrate surface crystal lattice begins to undergo elastic deformation. When the substrate elastic limit (load carrying capacity) is exceeded, dislocations form and plastic deformation begins.

Figure 10 shows that the fixed boundary barrier effect increases with both speed (50 and 100 m/s) and indentation depth. Because of the fixed boundary barrier, some dislocations start to slide away from the surface. As the indenter continues moving into the substrate, the surface begins to undergo dislocation.

When the indenter depth reaches 2 nm (at 50 and 100 m/s), the barrier effect of the grain boundary layer becomes stronger. More significant dislocation occurs at the grain boundaries of the sliding surface around the indenter as well, and the number tends to increase. At an indenter velocity of 200 m/s, the crystal face inside the substrate generates partial dislocation, which aggregates to form a slip surface. However, there are fewer dislocations because there is less time for them to occur.
Therefore, there is better plasticity and also enough time for dislocations to take shape. But at high speed, atoms are pushed outwards during indentation by force and deformed. There is no time for dislocations to form, but the applied force damages the bonds between the atoms and more force is needed to break them. As can be seen in Figure 12, the maximum loads are 1400, 1100, and 900 nN at indentation speeds of 200, 100, and 50 m/s, respectively. The force displacement curve is also significantly higher for faster indentation.

Before the indenter makes contact with the substrate, the energy difference between indenters traveling at different speeds is insignificant. When the indenter first makes contact with the substrate atoms (at a displacement of around 10 ps), the energy curve moves upwards, as can be seen in Figure 11. Since there is not enough time for atomic diffusion, dislocations do not form, thereby leading the disruption of atomic bonds. Atoms begin to move towards areas not under pressure and energy is also absorbed by lower layers of atoms. The temperature of the substrate around a faster moving indenter also tends to rise.

In a 2-nm deep indentation simulation at 200 m/s, by the time the indenter stops, the temperature will also have risen significantly. However, in this case the substrate atoms have not had time to absorb enough energy to disrupt the atomic bonds. More kinetic energy was given to the atoms by the heavier load from the indenter. The atoms diffuse outwards more rapidly and the higher temperature also softens the substrate around the indentation.

3.3.2. Temperature Effect Analysis

When an indenter begins to make contact with the substrate, the atoms vibrate energetically. The temperature in the substrate rises and results in the rapid diffusion of atoms. Plastic deformation occurs as atoms are dislocated by sliding. In the 1 nm indentation simulation, increasing the speed of the indentation raises the temperature of the atoms at the contact surface, see Figure 11. Since there is not enough time for atomic diffusion, dislocations do not form, thereby leading the disruption of atomic bonds. Materials begin to move towards areas not under pressure and energy is also absorbed by lower layers of atoms. The temperature of the substrate around a faster moving indenter also tends to rise.

In a 2-nm deep indentation simulation at 200 m/s, by the time the indenter stops, the temperature will also have risen significantly. However, in this case the substrate atoms have not had time to absorb enough energy to disrupt the atomic bonds. More kinetic energy was given to the atoms by the heavier load from the indenter. The atoms diffuse outwards more rapidly and the higher temperature also softens the substrate around the indentation.

3.3.3. Load Capacity Analysis

During the indentation process, material dislocation formation and plastic deformation is seriously influenced by indentation speed. At low speed, the residual stress in the substrate atoms is slowly released and transferred. Therefore, there is better plasticity and also enough time for dislocations to take shape. But at high speed, atoms are pushed outwards during indentation by force and deformed. There is no time for dislocations to form, but the applied force damages the bonds between the atoms and more force is needed to break them. As can be seen in Figure 12, the maximum loads are 1400, 1100, and 900 nN at indentation speeds of 200, 100, and 50 m/s, respectively. The force displacement curve is also significantly higher for faster indentation.

Before the indenter makes contact with the substrate, the energy difference between indenters traveling at different speeds is insignificant. When the indenter first makes contact with the substrate atoms (at a displacement of around 10 ps), the energy curve moves upwards, as can be seen in Figure 12. The differences in indenter energy at different speeds begin to appear and the energy level represents atom stability. Since the indenter traveling at 200 m/s causes severe shock to the substrate atoms, they move outwards and the energy curve is significantly higher. At about 22 ps, it can be seen that the energy continues to rise, but the band declines slightly. When the material is elastically deformed, intense inter-atomic activity will lead to energy enhancement. As soon as the yield strength is reached, the energy is more relaxed. However, the material enters the plastic deformation state and the curve shows a sudden decline. After this, the speed energy curve goes on rising as indentation continues until it reaches the boundary and stops.
the structure soften and confused. In addition to the slip around the indenter, there is a significant amount of slip in material further away from the area of contact. In simulations of indentation to 2 nm, the amount of slip surrounding the indenter at system temperatures of 300, 500, and 700 K continues to accumulate. There is more slip inside the substrate as well. However, at 900 K, the amount of slip around the area of contact between the indenter and the substrate is no longer obvious. This is because the system temperature is high enough to damage the atomic structure. Moreover, the atomic bonds weaken and atoms diffuse outwards. Therefore, the ability of the material to resist deformation disappears and the atomic structure softens, which produces irregular shapes.

3.4. The Effect of Different Temperatures on Nanoindentation

3.4.1. The Multilayer Model Deformation Mechanism for Various Types of Indenters

In simulations of indentation to 1 nm, dislocation slip in the substrate material at 300, 500, and 700 K is mainly the result of the indenter load, see Figure 13. Slip is focused and distributed in the substrate around the area of contact between the indenter and the substrate. The amount of internal slip in the substrate is small and the system temperature has little effect. When the system temperature rises to 900 K, the kinetic energy between atoms rises. This causes that the atoms suffer shock, thereby leading
structure around the area of contact will also soften. The higher the temperature, the smaller the force needed to achieve the set indentation depth. Moreover, the higher the temperature of the system is, the greater the dynamic energy between the atoms is. This causes intense atomic movement so that the structure of the substrate is more chaotic. Therefore, partial structural defects are generated and the load capacity will decrease.

The system temperature causes initial energy changes before the indenter makes actual contact with the substrate.

3.4.2. Load Capacity Analysis
From Figure 14, it can be seen that the maximum load at temperatures of 300, 500, 700, and 900 K was 1100, 1000, 950, and 580 nN, respectively. Since temperature affects atomic kinetic energy, when the initial temperature of the system is high, the kinetic energy of the substrate atoms goes up and atomic mobility increases. Changes take place in atomic structure around the area of contact between indenter and the substrate. The higher the temperature is, the higher the amount of atom mobility is. The internal structure around the area of contact will also soften. The higher the temperature, the smaller the force needed to achieve the set indentation depth. Moreover, the higher the temperature of the system is, the greater the dynamic energy between the atoms is. This causes intense atomic movement so that the structure of the substrate is more chaotic. Therefore, partial structural defects are generated and the load capacity will decrease.

The system temperature causes initial energy changes before the indenter makes actual contact with the substrate.
surface, which shocks the atoms and the energy band shows instability. When the indenter contacts the substrate, at a displacement time of about 10 ps, the atomic shock state eases and the band stabilizes. As the indenter continues to move downwards the substrate atoms are pushed outwards and the atomic spacing is altered. This outwards movement of kinetic energy results in the formation of structural deformation. Moreover, energy continues to rise slowly. When the simulation is about to stop, at a displacement time of 25 ps, the strong adsorption energy causes the structure to undergo a dramatic change. That is the rapid increase of the stress value and energy. Although the initial energy values have differences, the curve bands are very similar under the condition of fixed indentation parameters.

4. Conclusions

Molecular dynamics indentation simulation experiments were carried out using a range of parameters: indenters of different shapes and size, different indentation speeds and temperatures. The results showed:

(1) In the cases of different shapes of indenter, since the area of contact between the substrate and the indenter increases, the atoms are more severely vibrated by energy. Therefore, the distribution of the amount of slip and the loading force by a 6-nm wide indenter was relatively more than that from the trapezoidal indenter. When the depth of the indenter increases, the affected areas increase. Therefore, the maximum loading carrying force and potential energy also increase.

(2) It was observed that Au and Cu show more slippage. The amount of slip appeared in the substrates is distributed unevenly because the bond energy between the atoms is lower. The amount of atomic flow is higher under pressure thereby leading the larger amount of slip.

(3) In the simulations of indentation of a multilayer model, it was found that the grain boundary layer impedes dislocation. The initial slippage accumulates at the first grain boundary, but when the grain boundary is disrupted by an increase in the depth of indentation, atoms begin to diffuse to the lower layer and the amount of slip changes.

(4) At an indentation speed of 200 m/s, plastic deformation is not formed from the dislocation slips, but the direct disruption of the bonds between the atoms.

(5) At an indentation temperature of 900 K, the slip amount around the indenter is no longer clearly evident. This is mainly because the atomic bonds have been weakened and there is outwards diffusion. Therefore, the surface structure of the material softens and indentation can be achieved with a smaller load.

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ORCID

Te-Hua Fang http://orcid.org/0000-0002-7032-3193

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