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Tool/Chip Interfacial Friction Analysis in Atomic Machining of Polycrystalline Coppers

Three-dimensional (3D) molecular dynamics (MD) simulation is performed to study the tool/chip interface friction phenomenon in machining of polycrystalline copper at atomistic scale. Three polycrystalline copper structures with the equivalent grain sizes of 12.25, 7.72, and 6.26 nm are constructed for simulation. Also, a monocrystalline copper structure is simulated as the benchmark case. Besides the grain size, the effects of depth of cut, cutting speed, and tool rake angle are also considered. It is found that the friction force and normal force distributions along the tool/chip interface in both polycrystalline and monocrystalline machining exhibit similar patterns. The reduction in grain size over-all increases the magnitude of normal force along the tool/chip interface, but the normal forces in all polycrystalline cases are smaller than that in the monocrystalline case. In atomistic machining of polycrystalline coppers, the increase of depth of cut consistently increases the normal force along the entire contact area, but this trend cannot be observed for the friction force. In addition, both higher cutting speed and more negative tool rake angle do not bring significant changes to the distributions of normal and friction forces on the interface, but both factors tend to increase the magnitudes of the two force components. [DOI: 10.1115/1.4028025]
Shen and Sun [21] examined the atomic-scale friction behavior of an infinite flat–flat contact between copper and the diamond surface, and suggested that the friction behaviors were independent of the sliding velocity in the wearless sliding regime. Yang and Komvopoulos [22] investigated the effects of velocity and tool tip geometry on sliding friction. It was found that the frictional force increased from 20 to 30 m/s as the sliding velocity increased from 1 to 100 m/s. Ye et al. [23] analyzed the mechanism of material removal, chip formation, and friction in the nanometric machining of monocrystalline copper. The overall coefficient of friction, being equal to the ratio of the cutting force to the thrust force, was reported to be 0.64. Fang and Weng [24] proposed 3D MD simulations to study the effects of tool geometry and processing resistance on the atomic-scale cutting mechanism. The coefficient of resistance, namely, the ratio of the cutting force to the thrust force, was found to vary from 0.4 to 1.2 as the half-conic angle of pin tool changed from 15 deg to 75 deg. Until recently, the research effort was progressed to investigate the detailed tool/chip interaction along the interface. Ji et al. [25] modeled the atomistic machining process of monocrystalline copper with MD simulation. The analysis of tool/chip interface revealed that the distribution patterns of friction force and normal force are actually more complicated than those classical friction models developed for macromachining.

Most existing literature on MD simulation of machining usually adopted monocrystalline materials as the work material [26] because they are much easier to be modeled in simulation. This practice is not consistent with the fact that the majority of crystalline materials are in the form of polycrystalline structures. To address this, Shi et al. [27] investigated how the grain size impacts the machining performance at atomistic level and found that significant smaller forces were required to cut the copper workpiece with the increase of grain size. Meantime, Shi and Verma [28] compared the machining performance in machining of a polycrystalline and a monocrystalline copper structure using MD method. It was found that smaller cutting forces are required to machine the polycrystalline than the monocrystalline structure for all conditions investigated.

In this research, the tool/chip interface friction in atomistic machining of polycrystalline copper structures is investigated, and the effect of grain size on friction is revealed. Meanwhile, the effects of machining parameters, such as depth of cut and cutting speed in polycrystalline machining, are also studied.

### MD Simulation Methodology

#### Model Construction

Figure 1 shows a schematic of the MD model for atomistic orthogonal machining of polycrystalline copper. The work material is of copper structure and divided into three different zones, namely, boundary layer, thermostat layer, and Newtonian layer [27,28]. The boundary atoms are fixed in position to hold the structure of the bulk system. The thermostat atoms are arranged to surround the Newtonian atoms to make the boundary temperature close to environment temperature. The periodic boundary conditions [29] are applied in the transverse (Z) direction to reduce the boundary effect. The diamond cutting tool is assumed to be infinitely rigid such that the relative positions between tool atoms are unchanged during the machining process. The workpieces for all cases have the identical dimension of $39.6 \times 21.6 \times 18.0$ nm$^3$, which consists of 1,247,591–1,290,253 atoms depending on the grain size of the polycrystalline structures and 1,320,000 atoms for the monocrystal structure. Three polycrystalline structures with different average equivalent diameters (12.25 nm, 7.72 nm, and 6.26 nm) are generated, and the corresponding structures consist of 8, 64, and 120 grains, respectively.

For the interaction between copper atoms, the EAM potential [30] can describe well the energies and geometries, which is a multiphysical potential energy function in the following form:

$$E_{\text{tot}} = \frac{1}{2} \sum_{ij} \Phi_{ij}(r_{ij}) + \sum_j F_i(\rho_i)$$

where $\Phi_{ij}$ is the short-range pair-interaction energy between atoms $i$ and $j$, describing the electrostatic contributions, $F_i$ is the embedding energy of atom $i$, and $\rho_i$ is the host electron density at site $i$ induced by all other atoms in the system. The related EAM potential parameter values are shown in Table 1.

Morse potential [31,32] is used to describe the interactions between copper atoms and carbons of the diamond cutting tool,

$$\varphi(r_{ij}) = D \left( e^{-2a(r_{ij} - r_0)} - 2e^{-a(r_{ij} - r_0)} \right)$$

where $D$ is the cohesiveness energy, $a$ is the elastic modulus, $r_0$ is the distance between the $i$th copper atom and the $i$th carbon atom in the cutting tool, and $r_0$ is the atom distance at equilibrium. The parameters for the Morse potential between copper–carbon atoms are: $D = 0.1 eV$, $a = 1.70 \times 10^{-10}$ m$^{-1}$, $r_0 = 2.22 \times 10^{-10}$ m [31,32].

In this work, Gear’s predictor–corrector method is adopted to simulate the positions, velocities and accelerations of atoms under displacement conditions [29]. Both truncated radius method and Verlet’s neighbor lists are applied to reduce the computation burden. The first relaxation phase is completed with 4000 time steps by controlling the bulk temperature at 300 K with an NVT ensemble [31], where $N$ represents the number of particles, $V$ represents volume, and $T$ represents temperature. Thereafter, the atomistic machining is simulated by moving the diamond tool by a small distance toward the negative X-direction at each time step. Finally, the tool is retracted and another 4000 time steps are simulated for the final relaxation. The time step of 1 fs is used in all cases. The cutting tool adopts negative rake angles. The cutting tool is initially placed outside the workpiece. The initial offset distance, namely the distance between the cutting edge and the workpiece in X-direction (see Fig. 1), needs to be carefully selected. The distance depends on the rake angle $\alpha$ and depth of cut $d$. To

#### Table 1: EAM potential parameters for copper–copper pair interaction [27,28]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice constant (10$^{-10}$ m)</td>
<td>3.62</td>
</tr>
<tr>
<td>Cohesive energy (eV)</td>
<td>−3.49</td>
</tr>
<tr>
<td>Bulk modulus (GPa)</td>
<td>137</td>
</tr>
<tr>
<td>C' (GPa)</td>
<td>23.7</td>
</tr>
<tr>
<td>C_{44} (GPa)</td>
<td>73.1</td>
</tr>
<tr>
<td>ΔE_{EC}−E_{EC0} (meV)</td>
<td>42.7</td>
</tr>
<tr>
<td>ΔE_{EC}−E_{EC0} (meV)</td>
<td>444.8</td>
</tr>
<tr>
<td>Stacking fault energy (mJ/m$^2$)</td>
<td>39.5</td>
</tr>
<tr>
<td>Vacancy: $E_v$ (eV)</td>
<td>1.21</td>
</tr>
</tbody>
</table>
Normal and Friction Forces Along Tool/Chip Interface. The interaction between the formed chip and tool rake face is critical to the formation of chip morphology, cutting forces, and other phenomena observed in machining. As mentioned above, it has not been well addressed by the existing literature on nanometric or atomistic machining. Most only consider the total friction effect in nanomachining or nanoscraping by regarding the total force in the tool movement direction as the friction force. However, that is too simplified to reveal the interaction along the tool/chip interface. In our study, the friction behaviors on tool rake face are determined by only considering the cutting forces exerted on the tool/chip interface using a two-step approach. First, the atoms in a thin surface layer of tool rake face are divided into multiple groups. To accurately calculate the force along the tool/chip interface during the atomistic machining process, the length of groups should be as small as possible, for example, \( L_1 \) is kept at 0.4 nm (slightly larger than one \( C \)-lattice constant of 0.3567 nm), and \( L_2 \) is kept at 0.8 nm, as shown in Fig. 2.

The force (denoted as \( F_m \)) of the \( n \)th group can be calculated by adding up the forces of individual atoms in the group, which are the direct outputs of MD simulation. Second, the friction and normal force on the rake face of each group can be evaluated according to the tangential and normal cutting force of the same group. Meanwhile, the total cutting force along the interface can be obtained by adding up the force components of all groups in different axial directions. To calculate the action force \( F_m \) of the \( m \)th atom group, the individual interaction force acting on the carbon atom \( i \) in the tool due to the surrounding copper atom \( j \) in the material should be computed first by differentiating the potential energy, and then the action force \( F_m \) can be obtained by summing all the interaction forces on the tool atoms of the \( m \)th group

\[
F_m = \sum_{i=1}^{N} \sum_{j} \frac{\partial \phi(r_{ij})}{\partial y}
\]  

(3)

where \( F_m \) is the cutting force of the \( m \)th group, \( n \) is the quantity of atoms in the diamond tool of \( m \)th group. The action force \( F_m \) in vector form can be obtained by summing all the interaction forces on the tool atoms of the \( m \)th group. For each carbon atom, the reaction forces should also be summed up among its neighbor atoms, the truncated radius method [29] is employed to reduce the calculation time.

Then, the total cutting forces of all groups along the interface can be obtained by following equations:

\[
F_{Tx} = \sum_{m=1}^{M} F_{mx}
\]  

(4)

\[
F_{Ty} = \sum_{m=1}^{M} F_{my}
\]  

(5)

where \( M \) is the quantity of groups at the tool/chip interface, \( F_{mx} \) and \( F_{my} \) are the tangential and thrust cutting force of the \( m \)th group, respectively.

In this work, we investigate the stress distributions including the friction and normal forces along the tool/chip interface by computing the cutting forces of each atom group defined along the tool/chip interface. It should be noted that the force profiles are equivalent to the stress profiles since the contact area of each atom group is identical. The positive directions of the friction and normal force are shown in Fig. 2. The friction force \( \tau \) and the normal force \( \sigma_n \) generated by the \( m \)th group can be obtained by the following equations:

\[
\tau = F_{my} \cos(-\theta) - F_{mx} \cos(90 \, \text{deg} + \theta)
\]  

(6)

\[
\sigma_n = F_{mx} \sin(-\theta) + F_{nx} \sin(90 \, \text{deg} + \theta)
\]  

(7)

Cutting Conditions for Atomistic Machining Simulation. To study the effect of machining parameters on the tool/chip interfacial friction, 14 cutting conditions are selected for MD simulation. The machining parameters of these cutting conditions are summarized in Table 2. By comparing cases C1–C4, the effect of different copper structures can be revealed. By comparing cases C3, C5, C6, and C9, insights about the role of depth of cut in machining polycrystalline copper can be obtained. Also, the effect of cutting speed can be analyzed by comparing cases C5 and C7, and the effect of tool rake angle can be illustrated by comparing cases C3 and C8.

Results and Discussion

Chip Formation. The snapshots of cases C1 and C3 are shown in Figs. 3 and 4, respectively. For the purpose of brevity, the machining processes for other cutting conditions are not provided here. It can be seen that there are pronounced differences among the results while cutting different copper structures. This indicates that the copper structure affects the chip formation and subsurface deformation of the machined surface. This can be attributed to the different deformation mode from dislocation movement to other mechanisms such as grain boundary sliding [27,28].

By measuring the contact length of tool/chip shown in the simulation snapshots for cases C1–C6, the comparison can be made in Fig. 5. It can be observed that the contact length of tool/chip interface (at the tool travel distance of 25 nm) increases with the increase of the grain size, as well as depth of cut.

Total Cutting Forces. The total cutting forces of all atom groups along the tool/chip interface during the cutting processes are obtained. The tangential and thrust forces are the two force components of interest in the orthogonal machining. Figures 6(a)–6(d) show the evolution of the two force components during the atomistic machining processes for cases C1–C4, respectively. The results from machining both polycrystalline and monocrystalline structures reveal the similar stick-slip phenomena as reported by Shimizu et al. [10]. Also, the ratio of tangential force and thrust force in cutting processes mostly varied from 0.7 to 1.85.

It can be seen that the total cutting forces vary to a great extent for different copper structures. The average cutting forces are...
obtained by averaging the fluctuating force values in the relatively stable cutting stage, and the results are shown in Fig. 7. As the grain size decreases from 12.25 nm to 6.26 nm, both the average thrust and tangential forces decrease substantially. The similar phenomenon was obtained by Shi et al. [27] while analyzing the cutting force exerted on all the tool atoms by the polycrystalline copper atoms. However, the cutting forces in polycrystalline machining at cases C2–C3 are all smaller than those in monocrystalline machining. Shi and Verma [28] confirmed that higher cutting forces are required to machine a monocrystalline structure than a polycrystalline structure. It also can be seen that the average ratio of tangential force to thrust force decreases from 1.33 to 1.25 with the reduction in grain size.

Effect of Grain Size on Friction. Figures 8(a) and 8(b), respectively, show the friction and normal force profiles along the tool/chip interface under cases C1–C4, when the cutting travel distance is 25 nm. As mentioned previously, cases C1–C4 have a monocrystalline structure, and grain sizes of 12.25, 7.72, and 6.26 nm, respectively. It can be seen in Fig. 8(a) that the profiles of normal forces under cases C1–C4 starts from a peak value near

---

### Table 2 Parameters for atomistic machining conditions

<table>
<thead>
<tr>
<th>Cutting condition</th>
<th>Copper structures</th>
<th>Depth of cut (nm)</th>
<th>Cutting speed (m/s)</th>
<th>Rake angle (deg)</th>
</tr>
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<tr>
<td>C1</td>
<td>Monocrystalline</td>
<td>2.0</td>
<td>500</td>
<td>−15</td>
</tr>
<tr>
<td>C2</td>
<td>Polycrystalline (grain size: 12.25 nm)</td>
<td>2.0</td>
<td>500</td>
<td>−15</td>
</tr>
<tr>
<td>C3</td>
<td>Polycrystalline (grain size: 7.72 nm)</td>
<td>2.0</td>
<td>500</td>
<td>−15</td>
</tr>
<tr>
<td>C4</td>
<td>Polycrystalline (grain size: 6.26 nm)</td>
<td>2.0</td>
<td>500</td>
<td>−15</td>
</tr>
<tr>
<td>C5</td>
<td>Polycrystalline (grain size: 7.72 nm)</td>
<td>1.5</td>
<td>500</td>
<td>−15</td>
</tr>
<tr>
<td>C6</td>
<td>Polycrystalline (grain size: 7.72 nm)</td>
<td>2.5</td>
<td>500</td>
<td>−15</td>
</tr>
<tr>
<td>C7</td>
<td>Polycrystalline (grain size: 7.72 nm)</td>
<td>1.5</td>
<td>200</td>
<td>−15</td>
</tr>
<tr>
<td>C8</td>
<td>Polycrystalline (grain size: 7.72 nm)</td>
<td>2.0</td>
<td>500</td>
<td>−30</td>
</tr>
<tr>
<td>C9</td>
<td>Polycrystalline (grain size: 7.72 nm)</td>
<td>8.0</td>
<td>500</td>
<td>−15</td>
</tr>
</tbody>
</table>

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![Fig. 3 Snapshots of atomistic machining for case C1 at tool travel distance = (a) 15 nm and (b) 25 nm](image1)

![Fig. 4 Snapshots of atomistic machining for case C3 at tool travel distance = (a) 15 nm and (b) 25 nm](image2)
the tool cutting edge, sharply decreases, and then gradually decreases to zero at the point where the tool/chip contact no longer exists. The similar pattern was obtained at macroscale by Usui and Takeyama [33] in machining of lead with a photoelastic tool at 0.018 m/min. Also, it can be found that the magnitudes of normal forces are not significantly dependent on the grain size, but the reduction in grain size overall decreases the normal force along the tool/chip interface with only a few exceptions.

Figure 8(b) reveals the friction force profile along the tool/chip interface. For each case, the friction force starts a negative value near the cutting edge, increases to the maximum value at a small distance from the cutting edge, and decreases to zero as the contact between tool and chip ceases to exist. Interestingly, the similar patterns are found in macromachining results of literature, such as Baqgchi and Wright [34] in machining of steel tubes with a single crystal sapphire tool, and Chandrasekaran and Kapoor [35] in machining of lead with −10 deg rake angle tool at cutting speed of 0.0254 m/min. In the first atom group of the tool/chip interface...
As shown in Fig. 2, the friction force profiles for the monocrystalline and polycrystalline structures all exhibit negative values. This is because the material atoms below the cutting tool undergo extremely high pressure, the deformed chip atoms near the cutting edge have a tendency to move downward along the rake face due to the higher compression ahead of the tool. Meanwhile, in the first section of interface which is close to the cutting edge, both the friction and normal forces in monocrystalline machining are higher than that in polycrystalline machining.

Figure 9 shows that the profiles of the friction coefficient are also affected by grain size. The overall trends are still similar. With the increase of the distance from the cutting edge, the friction coefficient steadily increases, reaches the maximum in the middle part of the contact length, and then fluctuates around 0.8 to the point where tool/chip contact no longer exists.

Effect of Depth of Cut on Friction. Figure 10 depicts the effect of depth of cut on the normal and friction force distributions by comparing cases C5, C3, C6, and C9, which have the depths of cut of 1.5, 2.0, 2.5, and 8.0 nm, respectively. In particular, case C9 is simulated to study the tool/chip force distribution pattern when the depth of cut is higher than the average grain size, which is 7.72 nm in this case. The four cases adopt the identical cutting parameters except for the depth of cut. The results are obtained at the tool travel distance of 15 nm. It is observed that in general the change of depth of cut does not bring significant differences to the patterns of normal or friction stress profile. For the normal force profiles, the trends are similar, which all exhibit a peak near the tool tip, and decrease gradually toward zero at the end of tool/chip contact. Meanwhile, the magnitude of normal force over the entire contact length increases with the depth of cut. It should be noted that the increase of depth of cut to 8 nm does raise the entire profile of normal force to a much higher level. In terms of friction force patterns, the increase of depth of cut makes the friction force lower for the initial portion of contact length, while it makes the friction force higher for the later portion of tool/chip contact. Meanwhile, the increase of depth of cut does not bring significant increase to the peak friction force (compared with the normal force). Therefore, the depth of cut effect is more complicated for the interfacial friction force. The observation that the friction force is less sensitive to the change of depth of cut needs to be further investigated in the future.

Figure 11 compares the distributions of the friction coefficient under the three levels of depth of cut. The general trends of friction coefficient are similar under different depths of cut. The friction coefficient in the stable stage for all four cases varies in the range of 0.7–2.0. However, in the first half contact area, the friction coefficient appears to be higher when a smaller depth of cut is applied. It should also be noted that when the depth of cut reaches 8.0 nm, the friction coefficient is overall smaller than the other cases.

Evolution of Friction With the Progress of Machining. Figure 12 depicts the friction analysis results at the tool travel distances of 15, 20, and 25 nm for case C3. It can be observed that the normal force distributions at all three travel distances follow the same pattern, but the normal force overall becomes higher.
with the progress of machining. Also, the shapes of friction force curves are similarly shaped and the magnitudes of friction forces near the cutting edge are surprisingly identical. Figure 13 shows the friction coefficient distributions along the interface with the progress of machining. The shapes of curves of friction coefficient distributions are not strongly influenced by the travel distance and all reach the maximum at a distance of 4.4 nm from the tool cutting edge.

**Effects of Machining Speed and Tool Rake Angle.** Figure 14 compares the friction behaviors along the tool/chip interface in polycrystalline machining for cases C5 and C7, which have the cutting speeds of 500 and 200 m/s, respectively. It can be seen from Fig. 14(a) that as the cutting speed reduces from 500 to 200 m/s, the normal force becomes smaller when the distance from the cutting edge below 3.6 nm in polycrystalline machining, but it reverses the trend beyond that distance. The same observation can be made for the friction force profiles in Fig. 14(b). However, it is clear that the overall machining force for case C5 is still much higher than that of case C7. This is because the major contributor of overall cutting force is the first half of normal force profile, in which the force magnitude is significantly higher than the latter half of normal force profile, as well as the entire range of friction force profile.

Figure 15 illustrates the effect of tool rake angle on friction distribution by comparing cases C3 and C8, which adopt the rake angles of −15 deg and −30 deg, respectively. It can be seen that the shape of normal force distribution is not significantly affected by the tool rake angle in polycrystalline machining. The value of normal force near the tool edge slightly increases as the rake angle changes from −15 deg to −30 deg. The same phenomenon can be found in the friction force distributions even though more variations exist among friction force distributions obtained using the rake angle tools.

**Further Discussion**

It is well known that a number of friction models for tool/chip interface in machining operations have been developed in
literature. These models are usually obtained for some particular machining conditions (e.g., work and tool materials and cutting parameters). The famous ones include the constant Coulomb friction model, sticking–sliding model, constant shear friction model, and variable shear friction model [36]. In the traditional numerical simulation of machining (e.g., finite element analysis), some particular friction model needs to be assumed so that the simulation can be carried out. Nevertheless, the assumption of friction model could be problematic without enough consideration. MD simulation demonstrates its advantage in this aspect—it does not assume the friction model, and the computation results directly reveal the friction phenomena. Furthermore, it is clear that none of the above mainstream friction models for macromachining can provide a good fit for the friction distribution patterns obtained for atomistic machining of polycrystalline copper.

It should be noted that the machining speeds adopted in this study are significantly higher than the speed range for high speed machining. This is certainly the limitation of most MD simulation studies. The 200 m/s cases take more than 40 h to finish the computation using a cluster of 16 central processing unit (CPU) cores. The reduction of machining speed to the range of 1–10 m/s requires will have to use hundreds of CPU cores so that the computation can be completed within a reasonable amount of time. In the future efforts, we plan to explore the opportunities of graphics processing unit computing, which is believed to be effective for MD simulation with a much lower cost figure.

Also, in this study, a negative rake angle is chosen for all the cutting conditions. It is because at nanometric or atomistic scale, the rake angle is usually negative due to the tool edge radius. However, it will be beneficial to investigate the positive rake angle situation so that a more complete picture about friction mechanisms of nanometric or atomistic machining can be obtained. Finally, the validation of MD simulation results should be addressed. This experimental validation of any nanometric or atomistic machining has been a major challenge [26]. With the increase of simulation problem size, AFM scratching, AFM nanoindentation, and TEM in situ indentation are the possible techniques that can be adopted to verify the MD simulation models.

Conclusions

This paper investigates the friction behaviors along tool/chip interface in atomistic machining of polycrystalline copper structures. Besides the grain size, the cutting parameters of depth of cut and cutting speed are considered as well. Based on the simulation results, the following points can be summarized.

- The normal stress profiles in both polycrystalline and monocristalline machining at atomistic scale are all similarly shaped. The normal stress always starts from the maximum around the tool cutting edge, but it continuously decreases to zero at the end of tool/chip contact.
- The shear stress profiles follow a similar pattern for all the simulation cases. The shear stress always starts from a negative value near the cutting edge. This is because the material atoms below the cutting tool undergo extremely high pressure, and the deformed chip atoms near the cutting edge have a tendency to move downward along the rake face. The shear stress increases along the rake face and reaches a peak value. After that, it gradually falls to zero as the tool/chip contact ceases.
- The trends of normal force and friction force profiles are not significantly affected by the grain size of polycrystalline copper. However, the reduction in grain size increases the magnitude of the normal force along the tool/chip interface.
- In polycrystalline machining, the increase of depth of cut consistently increases the normal force along the entire contact area, and tends to increase the friction force for the majority of the tool/chip contact area. This is mainly because the cutting forces usually increase with increase of depth of cut.
- In polycrystalline machining, the normal and friction forces generally increase as the cutting speed and the magnitude of negative tool rake angle increase within the investigation range of this study.

References


