Atomic simulations of nanoscale friction behavior in polycrystalline alloy 690

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Abstract

Fretting wear is one of the most important failure forms of alloy 690 heat exchanger tubes in nuclear power plants. The key to understanding the fretting wear of alloys lies in the friction process, especially at the atomic scale. In this study, molecular dynamics simulations were performed on alloy 690 to investigate the nanoscale friction behavior and its influencing factors, laying a foundation for further understanding the fretting wear mechanism of alloy 690. The friction processes of a single-asperity (probe) on a smooth polycrystalline surface (matrix) were investigated by molecular dynamics simulations at the atomic scale, and the variation law of friction force during the friction process was calculated. The factors that affected the friction force were discussed, including the pressing depth, temperature, and sliding speed of the probe, and the friction force was positively correlated with the pressing depth and sliding speed of the probe, while the temperature had little effect on the friction force. Observations of the generation and evolution of dislocations during the friction process and related factors such as grinding grooves and wear debris were also reported.

1. Introduction

Wear, mainly in the form of fretting wear, is one of the most important failure forms of alloy 690 heat exchanger tubes in nuclear power plants, and many studies have been conducted on the wear of alloy 690 materials. Jae et al [1] conducted fretting tests on alloy 690 tubes and studied their fretting wear mechanism under room temperature. Guo et al [2] studied the influence of different damping rod materials on the fretting wear of alloy 690 heat exchanger tubes, while Yun et al [3] explored the influence of oxide film formation on the wear performance of alloy 690 tubes. Recently Zhang et al [4] investigated the fretting wear behaviors of Inconel 600 and 690 plates against 304 stainless steel ball in pure water. The above articles and other similar reports have shown that the key to understanding the wear of these alloys lies in the friction process. In fact, fretting wear includes many mechanisms, including abrasive, adhesive, and corrosion wear, of which abrasive and adhesive wear will be produced during the friction process [5, 6]. Vanossi et al [7] summarized research progress on tribological phenomena in recent years and noted that the actual origin of friction was at the atomic scale; thus, the study of friction at the atomic scale has become increasingly important. The friction process and friction force can be observed with a friction force microscope (FFM) [8, 9]. Kizuka et al [10] revealed structural variations in the atomic arrangements of two gold tips during approach, contact, bonding, and separation. Lang et al [11] used calibrated atomic force microscopy to describe the atomically frictional behavior of graphene under different relative humidity values. Molecular dynamics (MD) simulations have also been used as an effective method to explore the mechanism of nanoscale friction, and the use of MD in nano-tribology was proposed by Vargonen [12]. Zhu et al [13] carried out MD simulations with zirconium as the research object, and the results showed a frictional mechanical response with continuous fluctuations between the fretting interfaces. In addition, the simulation conditions have also been shown to exhibit an important influence on the
friction process [14–16]. Very recently, Zhu et al [17, 18] studied the friction and wear mechanisms of the nanocrystalline coating and single crystal of the nickel-based superalloy by means of molecular dynamics simulations. Shi et al [19] reported the friction and wear properties of Cu/Ta bilayer and multilayer during nano-scratch process. Hua et al [20] showed that the amorphous/amorphous nano-laminates have significant nano-scratch performance.

In this work, the friction mechanism of alloy 690 was investigated using MD simulations. To study the effects of grain boundaries on the friction force, a polycrystalline model was adopted in our simulation model. The law of friction force and the effects of probe pressing depth, temperature, and sliding speed on friction were studied. In addition, we focused on the generation and evolution of dislocations during the friction process, and the characteristics of the grinding groove and wear debris during friction were also described.

2. Methods

Single-asperity contacts have been widely considered the fundamental building blocks of friction, as noted in well-established interfacial models [21, 22]. In this work, we adopted a single-asperity and smooth polycrystalline model, and the simulation model is shown in figure 1. The single-asperity (probe) consisted of a rigid hemisphere, composed of a Fe-13Cr alloy (SUS 405 ferrite stainless steel) with a diameter of 4 nm. The object below the single asperity was the smooth surface of the polycrystalline matrix in the Ni-Fe-Cr alloy with a face-centered cubic lattice structure, and the molar fractions of Ni, Cr, and Fe were 0.6, 0.3, and 0.1, respectively. The size of the matrix was set to be 100 a × 30 a × 30 a with a lattice parameter a = 0.3524 nm to ensure that the influences of boundary conditions are excluded and the underlying atoms are not affected by the motion of the probe. The Atomsk software [23] was used to build the polycrystalline matrix model which contained four grains with an average grain size of 984.67 nm³. Firstly, the pure Ni polycrystalline matrix was constructed, a few Ni atoms were randomly replaced by the Fe and Cr atoms at a certain proportion, and then the probe model was constructed in the same way. Periodic boundary conditions were applied along the x- and y-directions, and free boundaries were applied along the z-direction. The matrix was divided into two parts according to their motion characteristics, which consisted of a boundary layer (0 ~ 1 nm) and freely deforming layer (1 ~ 10.572 nm). The simulations were performed using the NVT (constant-volume, constant-temperature) ensemble, so that the freely deforming layer was also the constant-temperature layer. The Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [24] software was used for friction simulations. Before the probe moved, the atomic coordinates were iteratively adjusted to minimize the energy, and the system was relaxed for t = 20 ps to reach the thermal equilibrium state, while the MD time step was set to Δt = 1 × 10⁻² ps. The interatomic interaction potential consisted of the embedded atom method (EAM) potential developed by Zhou et al [25], as this potential model could well describe Fe-Ni-Cr alloys in ferrite and austenite phases.

The sliding process in this MD simulation work consisted of two stages. The first stage applied a speed v_z to the probe in the negative z-direction, pressing it to depth d, while the second stage applied a constant speed v_x to the probe in the forward x-direction, and sliding it to the right.

3. Results and discussion

3.1. Formation of wear debris

During the probe sliding simulations, we observed that a large number of atoms accumulated on the surface of the matrix, as shown in figure 2. The pressing and sliding of the probe on the soft surface generated force that...
pushed the matrix atoms around the probe, as well as forces that separated the adhesion contact area, which caused the migration of matrix atoms. These atoms grew along the surface of the matrix and formed wear debris. Figure 3 shows the increase in the number of atoms in the debris during sliding of the probe, where $d = 0.3 \text{ nm}$, $v_x = 1.0 \text{ nm ps}^{-1}$ and $T = 300 \text{ K}$.

The number of wear debris atoms differed at various temperatures $T$ and pressing depth $d$. Figure 4 shows that the number of wear debris atoms increased with increasing $d$ and $T$. As the indentation depth increased, the contact area between the probe and the matrix increased, and more matrix atoms were squeezed and deformed. As a result, the number of overflowing atoms increased. Temperature had a significant influence on the atomic number of wear debris. As the temperature increased, the matrix had more kinetic energy, and the interactions between the matrix atoms become weaker, resulting in the departure of surface atoms.

During friction, energy generated by the probe was used to move all of atoms, as well as create and move dislocations. This resulted in a large number of atoms escaping from the matrix, which formed not only wear debris but also a grinding groove. Figure 5 shows the morphology of the grinding groove after friction, where the corresponding values of $d$, $v_x$, and $T$ were $0.3 \text{ nm}$, $1 \text{ nm ps}^{-1}$ and $300 \text{ K}$, respectively.

### 3.2. Frictional force

The Amontons-Coulomb law of friction states that friction force consists of a force that resists relative motion between objects in contact, where the friction coefficient is the ratio of friction force to the normal force. In the simulation, the friction force $f_x$ and normal force $f_z$ were obtained by calculating the sum of the forces on all the
probe atoms in the x and z directions respectively during slip, according to:

\[ f_{x,i} = \sum_i f_{x,i} \]  

\[ f_{z,i} = \sum_i f_{z,i} \]  

where \( f_{x,i} \) is force on the \( i \)-th atom in the x-direction, and \( f_{z,i} \) is the force on the \( i \)-th atom in the z-direction. The coefficient of friction \( u \) could be obtained by the ratio of \( f_x \) to \( f_z \), according to:

\[ u = \frac{f_x}{f_z} \]  

Figure 6 shows the variations of \( f_x \) and \( u \) with pressing depths \( d = 0.3 \text{ nm and } 0.4 \text{ nm} \), at temperature of 300K and \( v_x = 1 \text{ nm ps}^{-1} \). The results for other conditions are shown in figure S1 and S2. The friction force fluctuated and increased overall during the friction of the probe (figure 6(a)). Because the pressing depths \( d \) were small, there was less contact between the probe and matrix atoms, and the friction coefficients were small. However, the friction coefficient increased when the probe passed through the grain boundary, especially under the condition of larger pressing depth (figure 6(b)).

To explore the effects of simulation conditions on the friction process, we calculated the time averages of friction force and friction coefficient,

\[ f_{x,av} = \frac{1}{N_t} \sum_{j=1}^{N_t} f_{x,j} \]  

\[ u_{av} = \frac{1}{N_t} \sum_{j=1}^{N_t} u_j \]  

where \( f_{x,j} \) and \( u_j \) are the friction force and the friction coefficient at time \( j \), correspondingly, and \( N_t \) is the number of time intervals.
The effects of $v_x$ and $d$ on the time average friction force are shown in figure 7. According to the adhesion friction theory developed by Bowden and Tabor [26], the friction force could be regarded as the sum of the resistance generated by the adhesion and furrow effects. The shear force and furrow force increased as the probe was pressed deeper, resulting in an increase in friction force. Figure 7 shows that the friction force increased as the probe slid faster.

To determine the actual contact area between the asperity and the matrix, the formula established by Luan [27] was adopted in this work, which denoted the relationship between the actual contact area and the pressing depth:

$$A = D_{sum} \int_{s}^{s+d} A(s)f(Z)dz$$

$$= D_{sum} \int_{s}^{s+k} A(s)f(s+k)ds,$$  \hspace{1cm} (6)

where $A$ denotes the actual contact area; $D_{sum}$ is the asperity number density of the rough surface; $A(s)$ indicates the functional relation between the actual contact area and deformation; $s$ is the amount of deformation, also known as the pressing depth, and $k$ is the initial distance between the asperity and the matrix.

According to formula 6, as the depth of indentation increased, the actual contact area expanded. A larger actual contact area produced greater shear resistance, while a greater pressing depth resulted in more wear debris atoms, which also increased the friction force. In summary, the friction force increased as the probe pressed deeper. These theories agreed with the results presented in figure 7.

When the probe sliding speed changed, the friction force changed accordingly. As the probe slid faster, the moving distance increased. As shown in figure 3, a longer moving distance resulted in a greater wear debris volume, which led to a larger resistance during the motion process. At the same time, the dislocations generated...
during the moving process spent less time away from the moving region, and the accumulation of dislocations in the delineated region strengthened the matrix material. Both effects could lead to a greater friction force. In conclusion, the frictional force increased when the probe slid faster, which was consistent with the results presented in figure 7.

The results of $f_{cav}$ and $u_{av}$ at different temperatures for $d = 0.3$ nm and $v_x = 1$ nm ps$^{-1}$ are shown in figure 8. The corresponding curves of the instantaneous values of $f_x$ and $u$ during friction progresses at different temperatures are shown in figure S3. The figure 8 shows that as the temperature increases, the coefficient of friction increases. The overall variation of the friction force with temperature was quite small. We can get the same conclusion from the simulated results reported by Zhu et al [18]. It should be noted that the simulations were performed at different temperatures in NVT (constant-volume, constant-temperature) ensemble, which means the frictional heat was not concerned since the temperature was constant during a simulation of friction.

The friction force of the material can usually be described by the sum of the adhesive shearing force and the ploughing force [26], and this sum can be expressed in the following form:

$$f = K + P = A\tau_b + S\rho_e,$$

(7)

where $f$ is the friction force; $K$ is the adhesive shearing force and $P$ is the ploughing force. $K = A\tau_b$ in which $A$ is the adhesive area and $\tau_b$ is the shear strength of the adhesive joint. $P = S\rho_e$ in which $S$ is the ploughing area and $\rho_e$ is the ploughing force per unit area. For metal friction pairs, the value of $P$ is usually much smaller than the value of $K$, so the adhesion theory believes that the shear effect is the main reason for the friction force. High temperatures are typically conducive to liquid-like flow behavior of the alloy. As the temperature increased, the matrix material became soft, causing $\tau_b$ to decrease. However higher temperature may lead to a larger volume of wear debris, which inevitably results in a larger adhesive area, thus $A$ becomes larger. The two opposing effects may cancel each other out. As for the ploughing force $P$, the $\rho_e$ is only related to the properties of the material itself, and for a given indentation depth the number of matrix atoms in contact with the probe is a constant, causing the same ploughing area $S$. As a result, it is indicated by the current simulation that the temperature has a small effect on the friction force comparing with the other simulated conditions. In terms of friction coefficient, the effect of wear debris is greater than that of thermal softening, the higher the temperature, the more wear debris is produced, and the debris will block the front of the probe which increases the coefficient of friction.

### 3.3. Dislocation evolution

During the friction process, force was applied to the atoms of the matrix by the probe, which led to the initiation of dislocation and the plastic deformation of matrix materials. The OVITO software and the dislocation extraction algorithm (DXA) [28] were used to analyze the dislocation formation during friction in this work. Snapshots of dislocations in the matrix alloy are shown in figure 9, while the density variations are shown in figure 10. Friction produced a variety of dislocations, including perfect, Shockley, stair-rod, Hirth, and Frank type defects. These dislocations were dominated by Shockley dislocations (figure 11). The number of dislocations was small when the probe was initially pressed into the matrix, though as the probe slid, a multiplication of dislocations was observed, and different dislocations connected to form a larger source of dislocations. The dislocation density increased linearly between $t = 1$ ps and 5 ps and reached its maximum at $t = 5$ ps, where the total length of dislocations at $t = 5$ ps was approximately 1852 nm. The dislocations could potentially annihilate when they slipped to the surface or when opposing dislocations met, while the reactions
between the dislocations could produce a new type of dislocation, and these effects caused a reduction in dislocation length. Therefore, after 5 ps, the dislocation density started to decrease and then slowly became stable, and the total length of dislocations at $t = 15$ ps was approximately 1162.92 nm.

It was shown in figure 6 that the friction force fluctuated up and down but generally increased during the friction process. These fluctuations were due to the adhere-slip effect during friction. As the probe pressed into the matrix, the number of atoms that adhered to the probe surface gradually increased, and the lattice of the matrix produced slip and defects. As shown in figure 10, the dislocation density continued to increase after 1 ps. Generally, the onset of plasticity will be governed by dislocation nucleation; thus, the deformation of the nickel alloy matrix changed from elastic to plastic at this time. When the probe slid horizontally, we observed adhesion and migration of the matrix atoms in contact with the probe, and the friction force increased due to adhesion.
and atomic resistance. As the amount of deformation increased, the adhered atoms separated from the probe. After the probe was released from adhesion, the friction force decreased, and adhesion occurred again. At the same time, the formation of dislocations during sliding led to the release of accumulated strain energy, causing an instantaneous reduction in the friction force. Under the combined action of dislocation and adhesion, the friction force fluctuated up and down.

During the sliding process of the probe, the matrix underwent plastic deformation with increasing friction force, and there were two main plastic deformation modes: slip and twinning, both of which required dislocation motion. Because most of the random grain boundaries were high-angle grain boundaries, they impeded the sliding of dislocations, causing dislocation blocks. The dense dislocations at the grain boundaries possibly impeded plastic deformation, resulting in an increase in the friction force and friction coefficient.

As indicated in figure 9, the matrix produced a large number of dislocations during friction. We found that the dislocations were mainly generated at the grain boundaries during probe sliding, and the formation process of some of these dislocations was analyzed. Figure 12 shows the dislocation evolution of a grain boundary in the polycrystalline matrix (the green atoms in the figure indicate the grain boundary atoms, while the blue atoms indicate dislocation atoms), where when the probe moved, defects occurred in the matrix. Due to high energy at the grain boundaries, linear dislocations initiated from the grain boundaries (figure 12(a)). Under the action of force, the length of the dislocation line continuously increased, and the different linear dislocations connected forming ring dislocations (figure 12(b)). These ring dislocations grew continuously (figure 12(c)), finally forming stable large ring dislocations (figure 12(d)).

The synthesis and decomposition of dislocations were observed during the friction process, where Shockley dislocations were first generated and then increased as the probe slid. Dislocation motion caused the meeting of two Shockley dislocations, and they combined to form a new dislocation, namely the stair-rod dislocation. The stair-rod dislocation synthesis process identified by the dislocation extraction algorithm (DXA) implemented in OVITO software is shown in figure 13, and the equation for stair-rod dislocation synthesis is given by formula 8:

\[
\frac{1}{6} [\overline{1}21] + \frac{1}{6} [2\overline{1}] \rightarrow \frac{1}{6} [110]
\]  

During dislocation evolution, dissociation was also observed. As shown in figure 14, a stair-rod dislocation dissociated into two Shockley dislocations.

4. Conclusions

In present work, MD simulations were performed to study the frictional sliding of a single-asperity on a smooth polycrystalline of alloy 690. It was observed that the overall friction coefficient was quite small but increased when it passed through the grain boundary. The friction coefficient increased with the increasing of temperature. The friction force increased with increasing pressing depth and sliding speed of the probe. Comparing with the friction coefficient, the temperature had less effect on the friction force. The number of wear debris atoms (volume of wear debris) showed an increasing trend during the friction process, and more debris atoms were observed with increasing probe pressing depth and temperature. Dislocations occurred...
mainly at the grain boundaries and then developed outward during the friction process, the dislocation density increased significantly before 5 ps, then decreased slowly and became stable, and different Shockley dislocations interacted to produce stair-rod dislocations.

Figure 12. Dislocation generation process during friction for $v_x = 1 \text{ nm ps}^{-1}$, $T = 300\text{ K}$ and $d = 0.3 \text{ nm}$: dislocation structures at (a) 8 ps, (b) 9 ps, (c) 10 ps, and (d) 11 ps.

Figure 13. Stair-rod dislocation synthesis under condition of $v_x = 1 \text{ nm ps}^{-1}$, $T = 300\text{ K}$ and $d = 0.3 \text{ nm}$: dislocation at (a) 8 ps, (b) 8.5 ps, (c) 9 ps, (d) 10 ps.
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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Conflicts of interest

The authors declare no conflict of interest.

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Figure 14. Decomposition of stair-rod dislocations into two Shockley dislocations under conditions of $v_s = 1 \text{ nm ps}^{-1}$, $T = 300 \text{K}$ and $d = 0.3 \text{ nm}$: a dislocation structure at (a) 11 ps and (b) 12 ps.
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