A molecular dynamics study of scale effects on the friction of single-asperity contacts

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The apparent scale effect on friction of single-asperity sliding was investigated with the aid of a molecular dynamics analysis. The specimen material used was mono-crystalline copper, while the asperity materials were diamond and copper, respectively. It was found that a friction transition does exist but depends on interface conditions between the asperity and specimen.

KEY WORDS: friction transition; scale effect; molecular dynamics; single asperity

1. Introduction

A micro-mechanical dislocation model of frictional slip between two asperities was presented by Hurtado and Kim [1], which predicts that the friction stress is constant and of the order of the theoretical shear strength, when the contact size is small. However, at a critical contact size there is a transition beyond which the frictional stress decreases with increasing contact size, until it reaches a second transition where the friction stress gradually becomes independent of the contact size. Hence, the mechanisms of slip are size-dependent, or in other words, there exists a scale effect. Before the first transition, the constant friction is associated with concurrent slip of the atoms without the aid of dislocation motion. The first transition corresponds to the minimum contact size at which a single dislocation loop is nucleated and sweeps through the whole contact interface, resulting in a single-dislocation-assisted slip. This mechanism is predicted to prevail for a wide range of contact sizes, from 10 nm to 10 μm in radius for typical dry adhesive contacts; however, there are no available experimental data in this size range. The second transition occurs for contact sizes larger than 10 μm, beyond which friction stress is once again constant due to cooperative glide of dislocations within dislocation pileups. The above dislocation model excludes wear or plastic deformation of either surface.

On the other hand, on the atomic scale, based on molecular dynamics modelling, Zhang and Tanaka [2] proposed a mechanism with four transition regimes, that is no-wear, adhering, ploughing and cutting regimes, when the radius of the asperity is kept constant but the depth of asperity indentation is increasing. In this case, the contact size increases due to the increment of the indentation depth of the asperity and thus both wear and plastic deformation consequently occur.

In the present study, a molecular dynamics simulation is carried out to analyze the mechanism of sliding when the asperity radius varies from 5 to 30 nm but the indentation depth is kept unchanged, so that any variance in the mechanisms of sliding is solely due to the different contact size. The molecular dynamics models consist of a single cylindrical asperity (rigid diamond and copper) of various radii, sliding across the face of a copper workpiece on its (111) plane with a speed of 5 m/s. The indentation depth, d, was 0.46 nm and -0.14 nm (0.14 nm above the workpiece), respectively, where d is the distance between the surfaces of the asperity and specimen defined by the envelopes at the theoretical radii of their surface atoms [2–4]. As usual [2–4], two layers of thermostat atoms are arranged around the Newtonian copper atoms of the specimen to ensure that the heat generated during sliding can conduct out of the control volume properly. The boundary atoms are fixed to the space to eliminate the rigid body motion of the copper specimen. The velocities of atoms in the initial configuration of the model follow the Maxwell distribution. The modified Morse potential used by Zhang and Tanaka in their simulation of sliding between a diamond tool and copper workpiece [2] was applied to describe the interactions between the atoms. The simulation model is shown schematically in figure 1. It must be noted that the molecular dynamics simulation cannot cap-

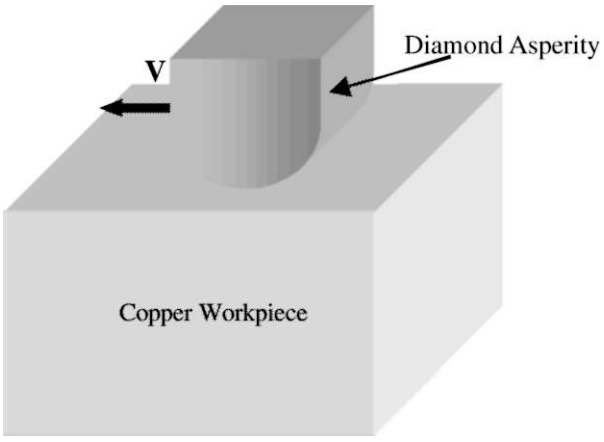

Figure 1. Simulation model of dry contact sliding between diamond asperity and copper.

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ture the second transition because it will require too long a computation time to analyse a model on the order of micrometers. Furthermore, the simulation is carried out under absolute vacuum conditions so that there will be no contamination on the surfaces of the asperity and workpiece.

2. Results and discussion

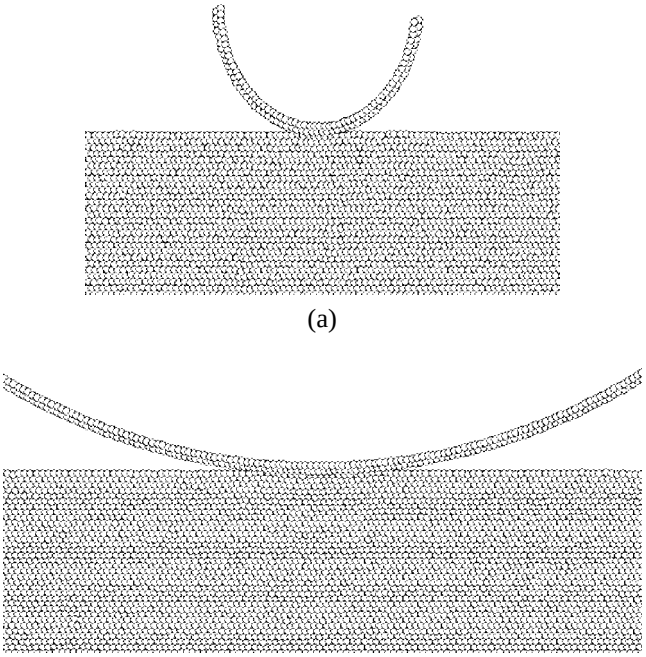
2.1. Sliding with a diamond asperity

2.1.1. Friction stress and workpiece deformation

Figure 2 shows snapshots of the simulation with different asperity sizes. It can be clearly seen that the depths of indentation in the simulations are small enough so that there are no dislocations created within the workpiece. The sliding simulations are all performed within the elastic no-wear regime described by Zhang and Tanaka [2].

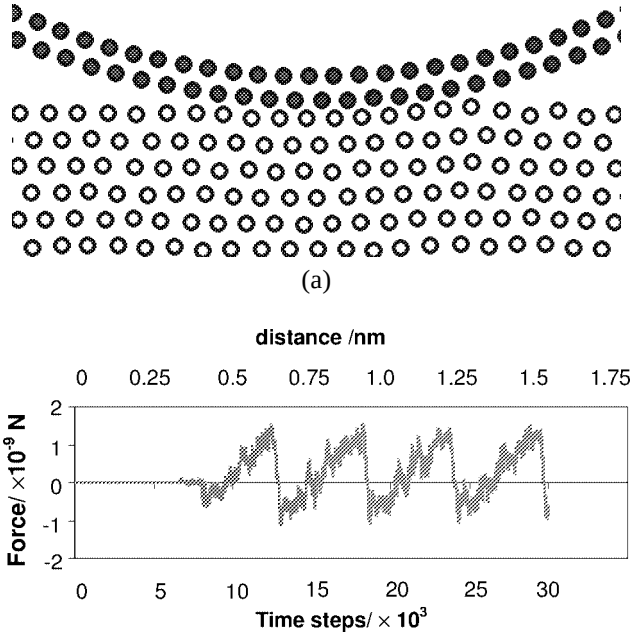
In the case where radius of the carbon (diamond) asperity is less than 12 nm, the carbon atoms slide across the copper atoms in close contact. The surface of the copper workpiece conforms closely to the shape of the asperity tip in contact (figure 3(a)). There is also strong indication of atomic stick–slip between the atoms of the asperity and the workpiece (figure 3(b)). This implies that the sliding mechanism involved is similar to the ideal slip of two atomic planes in a perfect dislocation-free crystal. Hurtado and Kim [1] referred to this sliding mechanism as concurrent slip. In addition, the friction stress averages around a constant value of 5 GPa, regardless of the contact width (figure 5).

In the case where the asperity radius exceeds 12 nm, there are considerable differences in the sliding mechanism involved. The surface of the copper workpiece does not conform closely to the shape of the carbon asperity (figure 4(a)) and there is little atomic stick–slip between the atoms of the asperity and the workpiece (figure 4(b)). In addition to that, the frictional stress now decreases with increasing contact width (figure 5). Hence, the friction stress is constant before the first transition but after which it decreases up on increasing contact width (by increasing the asperity radius). This clearly indicates a change in the mechanism of sliding.



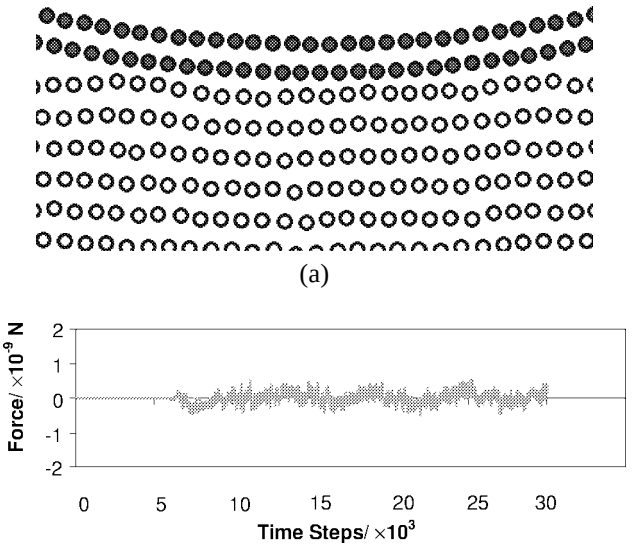
(a) (b)

Figure 2. (a) Snapshot of sliding simulation with 5 nm radius diamond asperity. (b) Snapshot of sliding simulation with 30 nm radius diamond asperity.



(a) (b)

Figure 3. (a) Surface of copper workpiece conforms closely to shape of asperity with radius 8 nm. There is good contact. (b) Stick–slip phenomenon in sliding for diamond asperity of radius 8 nm.



(a) (b)

Figure 4. (a) Surface of copper workpiece does not conform closely to the shape of the asperity with radius 30 nm. (b) No stick–slip phenomenon in sliding for asperity of radius 30 nm.

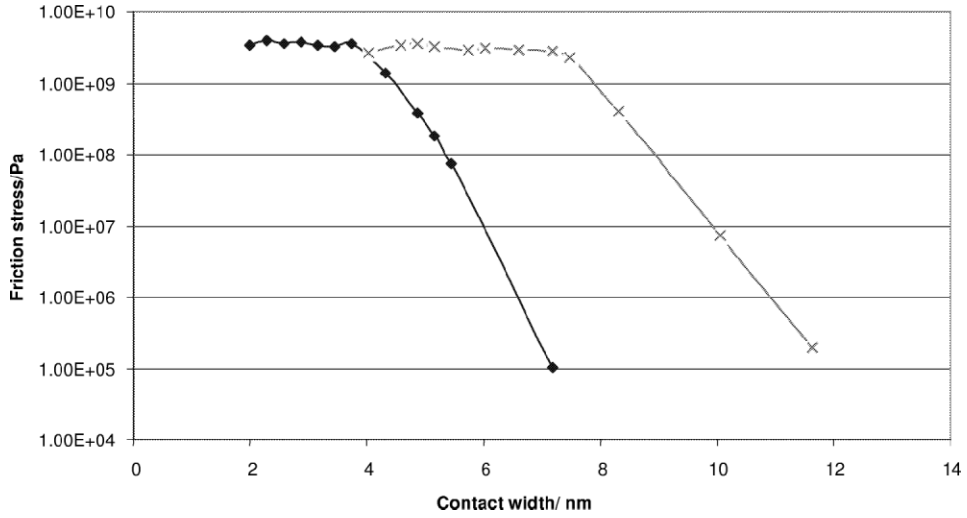


Figure 5. Frictional stress against contact width for indentation depths of (♦) −0.14 and (×) 0.46 nm.

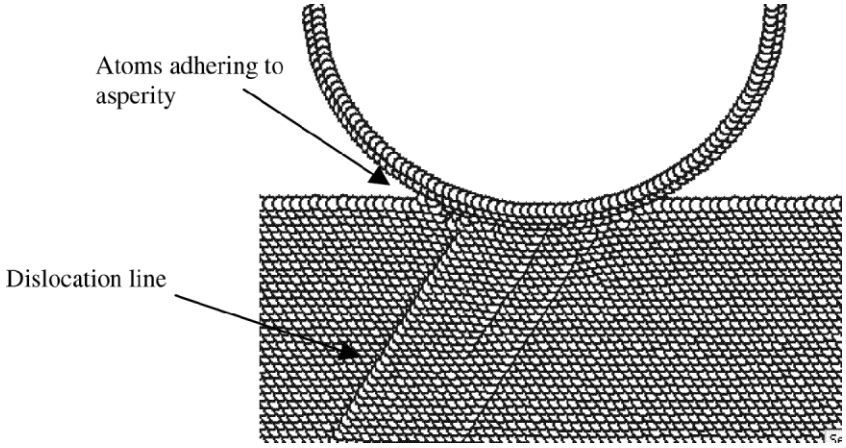


Figure 6. Sliding simulation with indentation depth 0.46 nm and asperity radius 5 nm.

At first sight, the change is in agreement with Hurtado and Kim [1], who proposed that, above a critical contact size, dislocations in the interface would be nucleated at the periphery of the contact, with a consequent reduction of friction with contact size. This question will be returned to in section 2.3.

When the depth of indentation is increased to 0.46 nm, a somewhat similar relationship between friction stress and contact width is obtained. Figure 5 compares the variation of the friction stress and the critical contact width at the first transition when the indentation depth changes. It is clear that the indentation depth influences both the critical contact size and the rate of friction reduction after the transition. At this greater indentation depth, however, figure 6 shows that permanent damage and wear are occurring. Dislocation lines indicating plastic deformation *within the body of the solid* are also visible. This behavior is similar to the adhering regime described by Zhang and Tanaka [2,3].

2.1.2. Contact width

The contact width between the asperity and workpiece obtained by the above molecular dynamics simulation can be compared with the predictions of the JKR theory, which shows, for the present configuration of a circular cylinder in contact with a half space (plane-strain), that the indentation load per unit width on the asperity, P, and the contact width, $2a$, follows the relationship of

$$P = \frac{\pi E^* a^2}{4R} - \sqrt{2\pi E^* a w}, \tag{1}$$

where R is the radius of the asperity, E^* is the effective modulus of the contact system [5] and w is the work of adhesion, which can be determined by a nano-indentation simulation using molecular dynamics analysis. It is found that for the present diamond–copper (C–Cu) system, $w_{\mathrm{C–Cu}} = 1.476\ \mathrm{J/m^2}$. Since we have assumed a rigid diamond asperity in the molecular dynamics simulation, the E^* in equation (1) becomes 125.36 GPa by taking $E_{\mathrm{C}} = \infty$, $E_{\mathrm{Cu}} = 110$ GPa and $\nu_{\mathrm{Cu}} = 0.35$ [7].

Table 1 compares the contact widths from the molecular dynamics simulation, the JKR theory of equation (1) and the Hertzian contact theory under various conditions. The values from the JKR and simulation are different, although the deformation of the copper workpiece at $d = -0.14$ nm was

Table 1
Contact lengths calculated by the JKR and MD analyses for the case of diamond–copper interactions.

	Contact length $2a$ (nm)	
	$d = -0.14$ nm, $P = 0.625$ N/m	$d = 0.46$ nm, $P = 22.969$ N/m
$R = 5$ nm		
JKR	2.914	3.764
MD	2.870	4.120
Hertz	0	2.160
	$d = -0.14$ nm, $P = 0.824$ N/m	$d = 0.46$ nm, $P = 27.34$ N/m
$R = 8$ nm		
JKR	3.99	5.152
MD	3.731	5.740
Hertz	0	2.980

purely elastic and that at $d = 0.46$ nm was almost purely elastic. A possible cause is that the contact width of the molecular dynamics simulation contains the effect of sliding, while equation (1) does not. It is also worth noting that the predictions by the JKR theory compared to the predictions by the Hertzian contact theory are much closer to the molecular dynamics results. This indicates that the effect of normal adhesion is considerable.

In calculating the contact width above using equation (1), the force P used is from the corresponding molecular dynamics simulation as listed in the table.

2.2. Sliding with a copper asperity

2.2.1. Friction stress and workpiece deformation

As a further development to the simulations done above, we used a copper asperity in the following analysis. Thus the interaction between the asperity and workpiece atoms was Cu–Cu. However, the copper asperity was still assumed to be rigid. This was done to investigate if the same slip mechanism would apply to the copper–copper sliding and whether the contact width obtained would approach those predicted by the JKR theory.

Results show that for an asperity of small radius (5 and 10 nm) the mechanism of sliding is similar to that of the case of small diamond asperity of radius less than the critical size, i.e., the atoms of the asperity slip concurrently over the workpiece atoms and the friction stress remains constant regardless of asperity size. The stick–slip phenomenon is also prevalent in the simulation (figure 7). Figure 8 shows a copper asperity of radius 5 nm sliding over a copper workpiece. The shape of the workpiece conforms closely to the shape of the asperity, implying concurrent slip. The friction stress is calculated to be 2.3 GPa. When the radius of asperity is 10 nm, the friction stress is also approximately 2.3 GPa. This is consistent with the theory of concurrent slip as the friction stress is independent of the contact width.

However, when the size of the asperity increases further (20 nm), plastic deformation of the workpiece almost invariably occurs (figure 9). This is due to the strong normal adhesion between the asperity and workpiece atoms. This phenomenon does not happen in the previous diamond–copper

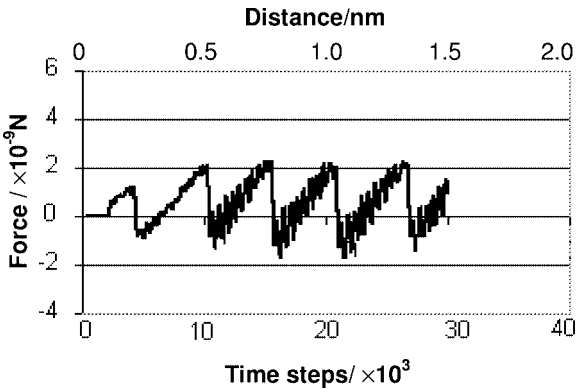


Figure 7. Stick–slip phenomena experienced by copper asperity of radius 5 nm.

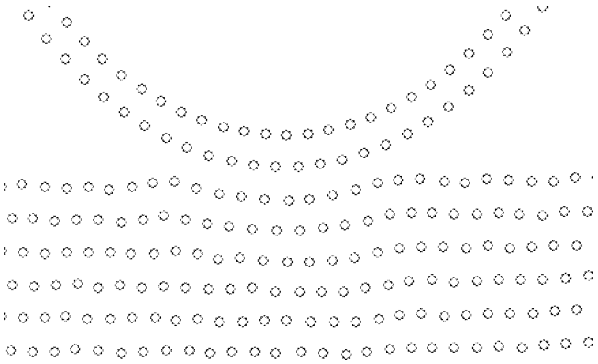
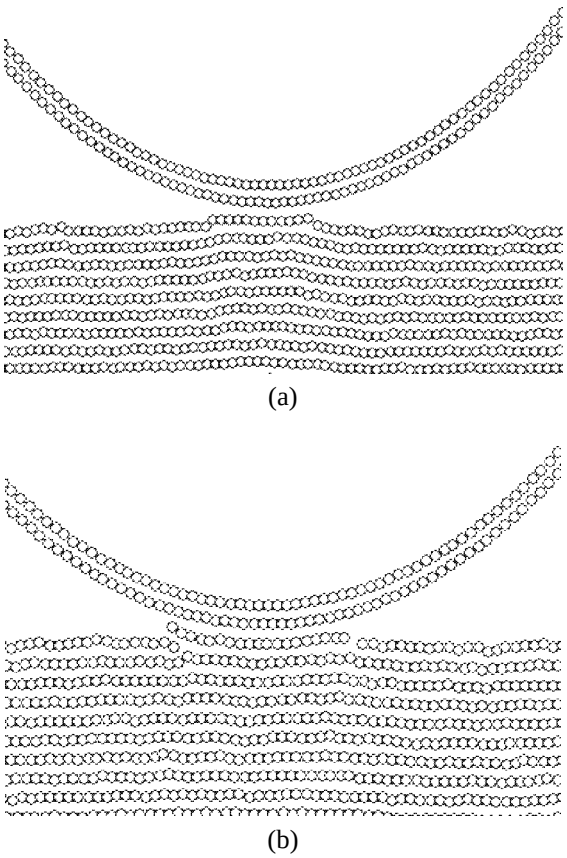


Figure 8. Atoms of radius 5 nm copper asperity sliding across workpiece concurrently at the indentation depth of −0.14 nm.

sliding because the C–Cu interaction is weaker. With the intervention of plastic deformation, the transition from concurrent slip to single-dislocation-assisted slip cannot be observed. Friction stress increases rather than decreases when the asperity radius changes from 10 to 20 nm.

2.2.2. Contact width

The work of adhesion for the copper–copper system, $w_{\mathrm{Cu–Cu}}$, is 1.960 J/m^2, also determined by a nano-indentation simulation using molecular dynamics analysis. Table 2 compares the contact widths calculated from molecular dy-



(a)

(b)

Figure 9. (a) Atoms in workpiece adhere to copper asperity (radius 10 nm) atoms at the indentation depth of −0.14 nm. (b) Plastic deformation of workpiece due to strong attraction between copper asperity (radius 20 nm) and workpiece atoms.

Table 2
Contact lengths calculated by the JKR and MD analyses for the case of copper–copper interactions when $d = -0.14$ nm.

	Contact length $2a$ (nm)
$R = 5$ nm, $P = 4.453$ N/m	
JKR	3.352
MD	3.731
$R = 8$ nm, $P = 6.76$ N/m	
JKR	4.656
MD	5.434
$R = 20$ nm, $P = 7.97$ N/m	
JKR	8.504
MD	7.150

namics with those from equation (1) at a fixed indentation depth $d = -0.14$ nm. When the asperity radius is 5 nm, the deformation in the workpiece is purely elastic, as shown in figure 8, and the molecular dynamics simulation matches the JKR result well. $R = 10$ nm seems to be a critical asperity size at which plastic deformation almost emerges, as can be seen from the locally raised surface atoms shown in figure 9(a). In this case, the contact width given by molecular dynamics is not in good agreement with that of the JKR. With $R = 20$ nm, however, local distortion of the surface atomic lattice becomes more severe and the local adhesion of atoms seems to make the contact width smaller (figure 9(b)). The JKR prediction then becomes much larger than that of the molecular dynamics.

Table 3
Quantitative comparisons of dimensionless shear stress (τ/μ) and dimensionless contact size (a/b) at transition.

	2D MD model		3D theoretical model
	$d = -0.14$ nm	$d = 0.46$ nm	
τ/μ	0.061	0.037	0.023
a/b	6.53	13.06	30
ξ (Pa/m)	2.90×10^{18}	1.46×10^{18}	1.88×10^{13}

2.3. A comparison with the dislocation model

Apparently, the above result of the molecular dynamics simulation is in agreement with the phenomenon predicted by the dislocation model [1], but the mechanisms are different, as pointed out in the discussion above. A quantitative comparison between the predictions of the two modelling methods is worthwhile, although the specimen materials are different and the dislocation model is three-dimensional whereas the present molecular dynamics simulation is two-dimensional. Table 3 shows the results of the dislocation model and those of the molecular dynamics simulation. The value of τ/μ obtained from the molecular dynamics simulation is close, particularly in the case of $d = 0.46$ nm, to that of the dislocation model, where τ is the shear stress and μ is the bulk shear modulus defined by Hurtado and Kim [1] as $\mu = 2G_1G_2/(G_1 + G_2)$ in which G_1 is the shear modulus of the asperity and G_2 is that of the copper specimen. In the present molecular dynamics simulation, the asperity is rigid so that $G_1 = \infty$ and $\mu = 2G_2 = 81.48$ GPa. The ratio a/b at the transition varies considerably with the indentation depth, where a is half of the critical contact width and b is the Burgers vector. The ratio for the case of $d = 0.46$ nm is closer to that of the dislocation model. However, it is interesting to note that in the transition zone the rates of friction reduction with contact size, $\xi = \mathrm{d}\tau/\mathrm{d}a$, are very different. The molecular dynamics analysis gives a much greater rate. The author is presently developing a three-dimensional model to try to achieve a better understanding.

3. Conclusions

For a sufficiently small contact, less than about 20 nm width, both the experiments of Carpick et al. [8], Lantz et al. [9] and the dislocation analysis of Hurtado and Kim [1] found that sliding occurs by concurrent slip of all the atoms in the contact at a frictional shear stress of the theoretical shear strength of the solid. Our molecular dynamics simulation supports this conclusion and displays the “stick–slip” behaviour expected with concurrent slipping. Above this critical contact size Hurtado and Kim predict that dislocations will be nucleated at the edge of the contact, with a reduction in frictional stress that is inversely proportional

to the square root of the size. Our results also show a reduction in friction above the critical size, but with a much greater sensitivity to size than in the 3D dislocation nucleation model. The critical size, while of the correct order of magnitude for dislocation nucleation, was found to vary with the degree of penetration of the asperity.

The contact sizes found in the molecular dynamics study were much greater than those predicted by the Hertz theory and broadly agreed with the JKR model for 2D contacts, using a theoretical value of the surface energy.

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