1 Introduction

In all problems of interest to tribology, surfaces need to first be brought into contact, before they can slide against each other and give rise to friction. Depending on the pressure exerted, the contact area that forms will depend on the surface topography, which is generally characterized by roughness over several length scales [1], and by the material properties.

Experimental flattening of a spherical asperity [2] as well as multi-asperities [3] shows that under moderate loading metal asperities undergo plastic deformation. This is to be expected also in the light of statistical friction models, which predict pressures exceeding the material hardness at low loads [4,5]. However, a clear understanding of the role of plasticity in the contact mechanics of metal surfaces is not yet reached. Plasticity in rough surface contact problems has so far been either neglected or modeled using the classical macroscopic continuum theory [6]. The shortcoming of continuum theory is that it cannot capture size effects in plasticity nor strain gradient effects. Since both of these effects are found to be dominant in the nano- and micro-indentation of metal surfaces [7–10], they are expected to be also relevant in the contact of rough metal surfaces, where each of the two surfaces act as a collection of nano and micro-indenters on the other.

For this reason, we set out to study plastic deformation of single and multi-asperity contacts in terms of DD plasticity, which can capture possible size and strain gradient effects, if present. This is possible because in the DD plasticity description dislocations are individually modeled. Besides the magnitude of the Burgers vector and multi-asperity contacts in terms of DD plasticity, which can capture possible size and strain gradient effects, if present. This is possible because in the DD plasticity description dislocations are individually modeled. Besides the magnitude of the Burgers vector and by the material properties.

Discrete dislocation (DD) plasticity simulations are carried out to investigate the effect of flattening and shearing of surface asperities. The asperities are chosen to have a rectangular shape to keep the contact area constant. Plasticity is simulated by nucleation, motion, and annihilation of edge dislocations. The results show that plastic flattening of large asperities facilitates subsequent plastic shearing, since it provides dislocations available to glide at lower shear stress than the nucleation strength. The effect of plastic flattening disappears for small asperities, which are harder to be sheared than the large ones, independently of preloading. An effect of asperity spacing is observed with closely spaced asperities being easier to plastically shear than isolated asperities. This effect fades when asperities are very protruding, and therefore plasticity is confined inside the asperities. [DOI: 10.1115/1.4030321]
where \( v_1 \) is the velocity of the rigid platen in the downward direction; \( w \) is the contact area per unit depth of the asperity. Outside the contact region, the top surface is traction free. The contact conditions are either frictionless

\[
\sigma_{12}(x_1, h + h_p) = 0, \quad x_1 \in \left[ \frac{L - w}{2}, \frac{L + w}{2} \right]
\]

(2)
or sticking

\[
u_1(x_1, h + h_p) = 0, \quad x_1 \in \left[ \frac{L - w}{2}, \frac{L + w}{2} \right]
\]

(3)
The reason for using both limiting contact conditions is that a sticking contact, contrary to a frictionless one, can induce contact shear stresses during flattening, since the horizontal displacement of the asperity is constrained. It is a priori unknown to which extent the contact shear stress induced during plastic flattening affects subsequent shearing, and therefore this is a matter of investigation in this study. The lateral boundary conditions are

\[
u_1 = \nu_2 = 0, \quad \text{for} \quad x_2 = 0 \quad \text{or} \quad x_1 = L
\]

(4)
The traction distribution along the contact normal to the platen determines the flattening force \( F_n \) (per unit of length). After flattening, shearing is imposed by prescribing the tangential displacement of the contact to be

\[
u_1(x_1, h + h_p) = v_1 dt, \quad x_1 \in \left[ \frac{L - w}{2}, \frac{L + w}{2} \right]
\]

(5)

\[
u_2(x_1, h + h_p) = u_0, \quad x_1 \in \left[ \frac{L - w}{2}, \frac{L + w}{2} \right]
\]

(6)

where \( v_1 \) is the velocity of the rigid platen in the horizontal direction, and \( u_0 \) is the flattening depth obtained after normal loading. The mean shear traction is denoted as \( \tau \). The bottom is fixed

\[
u_1 = \nu_2 = 0, \quad \text{on} \quad x_2 = 0
\]

(7)

2.2 DD Plasticity. The DD plasticity method by Van der Giessen and Needleman [16] is used, where further details of the formulation can be found. The stress, strain, and displacement fields of the dislocated crystal are calculated by superposing the elastic analytical solution for the dislocations in an infinite medium with the numerical image fields correcting for the boundary conditions. The evolution of dislocation structure in the crystal follows constitutive rules, which describe nucleation, glide, annihilation of dislocations, as well as pinning at obstacles. The simulations start from a dislocation-free state. The crystal contains dislocation sources and obstacles with average spacing \( L_{\text{nuc}} \) and \( L_{\text{obs}} \), respectively. Dislocation dipoles are generated when the shear stress on a source is larger than the nucleation strength, \( \tau_{\text{nuc}} \). There are two other parameters that are related to nucleation: the time, \( t_{\text{nuc}} \), required for formation of the dipole and the spacing between the newly generated dislocations, \( L_{\text{dis}} = Gh/2\pi (1 - \nu)\tau_{\text{nuc}} \), where \( G \) is the shear modulus, \( b \) is the magnitude of the Burgers vector, and \( \nu \) is the Poisson’s ratio. The glide velocity \( v' \) of the \( l \)th dislocation is proportional to the Peach–Koehler force \( f' \), according to \( v' = f'/B \) where \( B \) is the drag coefficient. The obstacles mimic small precipitates in the material that pin dislocations, as long as the resolved shear stress at the obstacles remains below the obstacle strength, \( \tau_{\text{obs}} \).

2.3 Material Parameters. The crystal is taken to have the elastic properties of aluminum with Young’s modulus \( E = 70 \text{ GPa} \) and Poisson’s ratio \( \nu = 0.33 \). Following Rice [17], the FCC crystal is modeled in two dimensions by considering three potentially active slip systems. In these simulations, the slip planes are oriented at \( \varphi = 15 \text{ deg}, 75 \text{ deg}, \) and \( 135 \text{ deg} \). This specific orientation is chosen to avoid alignment of the slip planes and any of the two loading directions, which would lead to unrealistic softening of the crystal. The sets of parallel slip planes form an angle of 60 deg with each other. This is a few degrees different from the real orientation of planes in an FCC crystal, as described in Ref. [17], but this difference will not noticeably affect our results. The spacing between slip planes in the crystal is 200 \( b \), where the magnitude of the Burgers vector being \( b = 0.25 \text{ nm} \). The average critical strength of the sources is taken to be \( \tau_{\text{nuc}} = 50 \text{ MPa} \), with a 20% standard deviation. The average source spacing \( L_{\text{nuc}} = 0.13 \mu \text{m} \), while the average obstacle spacing \( L_{\text{obs}} = 0.18 \mu \text{m} \), unless stated otherwise. The time span necessary for nucleation of a dislocation dipole, \( t_{\text{nuc}} \), is 10 ns.

The mesh is made of very fine \( 5 \text{ nm} \times 5 \text{ nm} \) elements at the surface of the crystal to accurately capture the contact traction distribution, while the mesh is coarser at the bottom of the crystal. Impenetrable obstacles are put at 0.02 \( \mu \text{m} \) underneath the contact to prevent exit of dislocations from the contact.

3 The Effect of Normal Loading on Plastic Shearing

3.1 Large Asperities. To investigate the effect of the applied contact pressure on the subsequent shearing, asperities with size

![Graph](image-url)
$w = 4 \mu m$ and $h_0 = 2 \mu m$ are first compressed to three values of the flattening depth, i.e., $u_2 = 0.0012$, 0.012, and 0.02 $\mu m$, and then sheared. Two different boundary conditions are applied on the surface of the asperity during flattening: the contact is either perfectly sticking or frictionless.

Figure 2(a) shows the evolution of the normal mean contact pressure, $P_m = F_n/w$, and the increase in total dislocation density $\rho$ (number of dislocations divided by the whole area of the crystal) during flattening of the asperity. The asperity behaves elastically until the flattening depth $u_2 = 0.006 \mu m$, when the first dislocations are nucleated, after which it gradually moves into a perfectly plastic response. The difference between the two contact conditions is small: the contact pressure for the frictionless contact is slightly lower than that for the sticking contact, while the total dislocation density is higher.

Starting from different flattening depths, indicated in Fig. 2(a) by the letters A, B, and C, the asperity is sheared up to $u_1 = 0.03 \mu m$ with perfect sticking contact conditions. Figure 2(b) shows that the shearing at the same displacement is easiest for the case of larger flattening depth (C). The effect of contact conditions on the shearing is negligible. The reason for this is that early plasticity in the asperity is assisted by the presence of the dislocations that were generated during flattening. The asperity that was not deformed plastically during flattening reaches a yield point of about 33 MPa and subsequently shears off at constant stress. The asperities that were plastically deformed during flattening do not show a yield peak, the shear stress increases gradually up to about 22 MPa.

In the following, we investigate if plasticity induced by flattening triggers a different plastic shearing mechanism than that occurring when shearing a dislocation-free crystal. Figures 3(a) and 3(b) show the stress state $\sigma_{12}$ and dislocation structure for the crystal that is flattened to $u_2 = 0.0012 \mu m$ (corresponding to point A in Fig. 2(a)) and on the right hand side the crystal flattened to $u_2 = 0.02 \mu m$ (corresponding to point C in Fig. 2(a)). The contact during flattening is in both cases frictionless. The asperity which is flattened deeper is characterized by a high dislocation density with numerous dislocations inside the asperity as well as in the subasperity region. Figures 3(c) and 3(d) show the stress state $\sigma_{12}$ after shearing to $u_1 = 0.01 \mu m$. For this tangential
that indicates shearing of the subasperity region. The bottom figures show two different mechanisms: plasticity in the crystal which is activated by the presence of dislocations in the vicinity of the contact. The plastic response is characterized by peaks caused by the presence of dislocations in the vicinity of the contact. The profiles obtained after shearing are shown in Fig. 4(b). The average contact shear stress is independent of the contact conditions used during flattening (frictionless or sticking); its average value is around 22 MPa, and even local differences are small.

We have shown that plastic flattening assists shearing of the asperities. What happens if the normal load is removed after flattening, before the shearing starts? To investigate this, asperities are first flattened to $u_2 = 0.012$ (B) or $0.02 \mu m$ (C) and then unloaded to points M and N, respectively, see Fig. 5(a). The residual amounts of deformation are about 0.0015 (M) and 0.008 $\mu m$ (N), respectively. The shear stress–displacement differences are negligible (see Fig. 6). This confirms that it is the presence of dislocations, not the presence of normal loading that assists plastic shearing.

3.2 Small Asperities. Simulations were also performed for a rectangular asperity, $w = 0.8 \mu m$, $h_0 = 0.4 \mu m$ with the same ratio as the large asperity to investigate whether there is a similar effect of preloading on the shearing of five times smaller asperities. In these simulations, the surface was kept sticking during flattening as the effect of contact conditions was found to be minor in Sec. 3.1. Notice that care must be taken in comparing the results with those for the large asperity above, since the elastic response is different.

Figure 4 shows the $\sigma_{12}$ stress profiles at contact after only flattening (Fig. 4(a)) and after flattening and shearing (Fig. 4(b)). The shear stress on the contact surface is zero everywhere for the frictionless contact. The plastic flattening facilitates shearing. This is because after flattening with a sticking contact and unloading, there is a remnant dislocation density in the crystal (see Fig. 6). This confirms that it is the presence of dislocations, not the presence of normal loading that assists plastic shearing.

3.3 Elastic Asperity on Plastic Substrate. To clarify the role of asperity plasticity, simulations are repeated for the small asperity $w = 0.8 \mu m$, after including an interface that is impenetrable to dislocations at the base of the asperity. The results are then compared with those in Sec. 3.2. Figure 9(a) shows the mean contact pressure as a function of flattening depth. As to be expected,

Figure 7(a) shows the mean contact pressure and the evolution of the total dislocation density. Dislocations started to nucleate at flattening depth of $u_2 = 0.003 \mu m$ and the asperity yielded at about $u_2 = 0.005 \mu m$. The small asperity is harder to flatten than the large asperity and fewer dislocations are nucleated compared with Fig. 2(a). In this paper, we will limit ourselves noticing that there is a size effect. The origin of this size effect is more complicated than dislocation starvation of the kind found for the tension specimen [18]. The main reason for the difference is that the load acting the asperity, but also a wide region underneath the asperity, where plasticity can occur. For more details about size effects in single asperities, the reader is referred to Ref. [19]. Figure 7(b) shows the shear stress as a function of tangential displacement. Shearing starts from different flattening depths as denoted by the letters A, B, and C on the curve in Fig. 7(a). Even though the contact shear stress at the final flattening depth is larger for larger preloading, the overall shearing response is independent of preloading within the expected statistical scatter for different realizations.

Figure 8 shows the stress state $\sigma_{12}$ and the dislocation distribution at various shearing displacement for small asperities flattened to $u_2 = 0.0012 \mu m$ (left hand side) and to $u_2 = 0.02 \mu m$ (right hand side). Despite a large number of dislocations nucleating during flattening (see Fig. 8(b)), they do not contribute to facilitate shearing, as evident from Fig. 7. Figures 8(c) and 8(d) are taken after shearing to $u_2 = 0.01 \mu m$. While the dislocation density and distribution appear drastically different, the response in terms of shear stress–displacement differs negligibly (see Fig. 7). This is a clear indication that the dislocation density, which is often calculated numerically or experimentally as a measure of plastic activity, bears little relation with it. Compared to the case of large asperity, the dislocation density in the asperity of Fig. 8(d) is four times as large. As a consequence, the active slip planes are highly populated with dislocations and the dislocation mobility is hindered. This is why in small asperities the dislocations are not available to glide and facilitate shearing.

**Fig. 4 The shear traction profiles $\sigma_{12}$ after (a) only flattening ($u_2 = 0.02 \mu m$ and $u_1 = 0 \mu m$) and (b) flattening and subsequent shearing ($u_2 = 0.02 \mu m$ and $u_1 = 0.03 \mu m$)**
elastic asperities require a larger contact pressure to be flattened. Figure 9(b) shows that upon shearing the shear stress is significantly affected by the properties of the asperity: If the asperity is elastic, a significant contribution to the asperity displacement arises from plasticity below the asperity and a much larger shear traction (about three times larger) is required to shear the elastic asperity by the same displacement. This indicates that plasticity inside the asperity is important in determining the global response of the system. However, even when the asperity is elastic, flattening has an effect on shearing, thanks to the mobility of dislocations in the subasperity.

4 Effect of Asperity Spacing

In this section, we investigate the effect of the spacing between asperities on the shearing response. In our previous study [12], we observed that it is more difficult to flatten a microscale sinusoidal asperity when it is surrounded by closely spaced asperities. Here, we will investigate whether a similar effect is found upon shearing. To this end, simulations are performed for a large single crystal of the type analyzed in Sec. 3, but with three asperities protruding from its surface spaced at $s_0$, as illustrated in Fig. 10. Simulations of flattening and shearing are performed on asperities with dimensions $w = 0.8 \mu m$ and $h = 0.08 \mu m$ spaced at $s_0 = 0.4 \mu m$, $s_0 = 2.0 \mu m$, and $s_0 = 8.0 \mu m$. The crystal has the same length of $L = 1000 \mu m$ and height $h = 50 \mu m$ as in Sec. 3. The pillars are initially flattened to a very small depth 0.0012 $\mu m$ to create contact but avoid dislocation nucleation, and then sheared with a constant velocity.

Figure 11(a) shows the contact shear traction of the middle asperity as a function of asperity shear strain. As illustrated in the inset of in Fig. 11(a), the asperity shear strain is defined as $\gamma = \frac{u'}{h'}$, where $h'$ is the height of the flattened asperity and $u'$ is the tangential displacement of the top of the asperity, and $u_0$ is the average tangential displacement of the base of the asperity. With the asperity strain defined in this way, the elastic response is almost independent of asperity spacing, and therefore the various cases are comparable. The results in Fig. 11(b) show a very pronounced asperity density effect; When asperities are rather isolated they are much harder to shear than when they are very close to each other. This is opposite to our previous findings on the flattening of asperities [12]: Increasing the asperity density hinders plastic flattening, while it is here found that it facilitates plastic shearing. The curve for $s_0 = 0 \mu m$ in Fig. 11(b) indicates the results for a single asperity whose width is equal to the size of the asperities, i.e., $w = 2.4 \mu m$.

Figures 12(a) and 12(b) show the stress state $\sigma_{22}$ and dislocation distribution at strain 0.008 for the most separated and closest asperities, respectively. Long “trains” of dislocations glide through the subasperity region in the case of closely spaced asperities, which does not happen for widely spaced asperities. Plastic shearing is a cooperative action of the three asperities and the material underneath.

Although the elastic shear traction–asperity strain response is almost independent of the spacing between asperities, the distribution of the shear stress in the crystal depends rather significantly

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**Fig. 5** (a) The mean contact pressure during flattening and unloading under sticking contact conditions for the asperity with $w = 4 \mu m$ and $h = 2 \mu m$. The letters B and C represent the points on the curves when unloading starts; M and N represent the points when the normal pressure disappears. (b) The contact shear traction at the contact as a function of tangential displacement during shearing from different dislocation distributions.

**Fig. 6** The stress state $\sigma_{22}$ and dislocation distribution for sticking contact when the asperity is totally unloaded from flattening depths: (a) $u_2 = 0.012 \mu m$ and (b) $u_2 = 0.02 \mu m$.
Fig. 7 (a) The normal mean contact pressure and total dislocation density during flattening under sticking contact conditions for a pillar with \( w = 0.8 \mu m \) and \( h_p = 0.4 \mu m \). The letters A, B, and C represent when the shearing starts. (b) The shear stress as a function of tangential displacement at different flattening depths.

Fig. 8 The stress state \( \sigma_{12} \) and dislocation distribution for the asperity with \( w = 0.8 \mu m \) and \( h_p = 0.4 \mu m \), on the left column is for the flattening depth \( u_2 = 0.0012 \mu m \) and on the right column is for the flattening depth \( u_2 = 0.02 \mu m \).
on it, as can be seen in Fig. 13. The region affected by loading closely spaced asperities is broad, so that dislocation nucleation can occur over a very wide region below the surface of the crystal. Based on our previous results on single asperity shearing [12], it is to be expected that slip in taller asperities is more confined to the asperities than to the region underneath. It is therefore interesting to see whether an effect of asperity spacing will be found for taller asperities.

To check if this is indeed the case, simulations are performed for taller asperities with \( h/w = 0.5 \) yet the same width \( w = 0.8 \mu m \). Figure 14 shows the shear traction as a function of shear strain for different spacings. The shear tractions are almost the same, indicating that there is no plastic interaction between tall asperities.

This is confirmed in Figs. 15(a) and 15(b) where the stress state \( \sigma_{12} \) and the dislocation distribution are presented for widely and closely spaced asperities at the shear strain \( \gamma = 0.03 \). Plasticity is mainly confined inside the pillar, although some dislocations appear in the bulk.

### 4.1 Effect of Normal Loading on Multi-Asperity Shearing

The preloading in the normal direction has been found in Sec. 3 to affect the shearing behavior of large pillars. In this
section, the effect of preloading on multi-asperities is investigated. Normal flattening was applied on asperities with size $w = 0.8 \mu m$ and $h_p = 0.08 \mu m$. The pillars are flattened to a depth of $u_2 = 0.02 \mu m$ and then sheared. Figure 16(a) for the shear stress as a function of shear strain shows that the asperity spacing effect is reduced by plastic flattening. This is because the isolated asperities become easier to shear thanks to the dislocations made available during flattening.

Similar simulations are performed for the taller asperities with $h_p = w = 0.5$. Figure 16(b) shows the shear stress as a function of shear strain for this protruding asperity. The spacing effect is absent and therefore independent of preloading.

5 Conclusions

DD plasticity simulations were performed to investigate the effect of flattening on the subsequent shearing behavior of asperities protruding from a large single crystal. If plastic deformation takes place upon shearing, the contact shear stress is reduced. This is relevant in determining the friction properties of the contact: If the contact shear stress is low, loss of adhesion at the contact is hindered. Our observations lead us to the following conclusions.

1. When large asperities, i.e., a couple of square micrometers, are flattened to $u_2 = 0.02 \mu m$, they deform plastically. The dislocations generated during flattening promote early plasticity upon shearing. At very small shearing displacement, the asperity is very compliant and the contact shear stress increases with increasing displacement without reaching the contact stress levels of asperities that were not preloaded.

2. Flattening smaller asperities to the same displacement, instead, does not affect subsequent plastic shearing. Despite there are many dislocations in the asperities, they are closely packed on a few active slip planes and therefore have smaller mobility.
An effect on asperity spacing is observed with closely spaced asperities being easier to plastically shear than isolated asperities. This effect is mainly triggered by the fact that shearing closely spaced asperities in the elastic regime gives rise to a wide region in the subasperity where the shear stress is large and therefore facilitates dislocation nucleation. This effect fades when asperities are very protruding, and plasticity mainly occurs inside of the asperities.

Acknowledgment

L.N. acknowledges support by the Dutch National Scientific Foundation NWO and Dutch Technology Foundation STW (VIDI Grant No. 12669). F.S. was supported by the Materials innovation institute M2i¹, Project No. MC2.06282.

References


Fig. 16 The shear stress as a function of shear strain at the flattening depth \( u = 0.02 \mu m \) for the asperity size: (a) \( w = 0.8 \mu m, h_p = 0.08 \mu m \) and (b) \( w = 0.8 \mu m, h_p = 0.4 \mu m \)

¹www.m2i.nl.