Plasticity under rough surface contact and friction
Plasticity under rough surface contact and friction

Proefschrift

ter verkrijging van de graad van doctor
aan de Technische Universiteit Delft,
op gezag van de Rector Magnificus prof. ir. K.C.A.M. Luyben,
voorzitter van het College voor Promoties,
in het openbaar te verdedigen op maandag 11 januari 2016 om 15:00 uur

door

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Introduction
1.1. General introduction

Friction arises when two metal surfaces in contact slide relatively to each other. The occurrence of friction is instrumental to many industrial processes as metal forming and deep drawing. Similarly, joining of surfaces through bolts strongly relies on friction. There are also many applications, however, where friction is detrimental, the most typical examples being bearings and machines with moving parts. It is estimated that if one could build a car out of frictionless components, fuel consumption could be reduced by 15% (Tung and McMillan, 2004).

Irrespective of whether friction is or not desired, there is a strong need for a better understanding and control of this phenomenon. Despite several efforts in this respect during the centuries, even the contact behavior of plastically deforming surfaces is not yet well understood. Indeed, even the most advanced statistical friction models neglect plasticity and describe the materials in contact as purely elastic (Müser, 2008; Persson, 2001).

The aim of this thesis is to gain a better understanding of plastic behavior during contact of rough metal surfaces by means of computer simulations. Seemingly smooth surface in contact (see the red circles in Fig. 1.1) are in fact characterized by roughness with a fractal nature. Addressing all the length scales involved is outside the scope of this work, here we will focus on the micro-scale, which is the scale at which size dependent plasticity is critical for metal behavior. The roughness of the surface is simulated as sinusoidal waves or pillar shaped asperities with different dimensions. Understanding the behavior of simple geometries paves the

![Figure 1.1: (a) The sketch of a deep drawing process and (b) a bolt connecting two metal sheets.](image-url)
way to the study of more complex real surfaces.

Given the rough nature of metal surfaces, the true contact area is only a fraction of the apparent contact area (Bowden and Tabor, 1950), as shown in Fig. 1.2b. While critical for better insight in the friction phenomenon, the change of true contact area and deformation of the asperities during contact loading cannot be tracked experimentally due to a significant limitation: the contact is currently inaccessible for characterization techniques.

This is probably why there is a very wide body of analytical and numerical work on contact. Studies of elastic contact were performed starting from the elastic contact of spheres (Archard, 1957) against a semi-infinite manifold to that of surfaces with different distributions of asperity heights, self-affine or Weierstrass surfaces (Campañà et al., 2008; Ciavarella et al., 2000; Putignano et al., 2012). The most advanced of these models, as the one developed by Persson and Müser (Müser, 2008; Persson, 2001) take into account elastic interaction, but are inappropriate to study plastically deforming surfaces.

Even a small mechanical load usually causes plastic deformation on contact asperities, for the resolved shear stress at the local contact is very large (Dieterich and Kilgore, 1996; Dwyer-Joyce et al., 2001).

Most of the current available contact models are based on the classical continuum theory of plasticity (Gao and Bower, 2006; Li et al., 2012; Majumdar and Bhushan, 1991; McGinty and McDowell, 2004; Roters and Zhao, 2002), which provides an appropriate description of contact between crystalline solids only if the
contacts are larger than several micrometers. Below this scale plasticity is size dependent, with smaller sized metal objects being harder to deform than large ones (Greer et al., 2005; Nicola et al., 2003; Volkert and Lilleodden, 2006). It is to be expected that micro-scale asperities on a rough surface will also display a size dependent behavior. To which extent this behavior will affect the contact pressure and contact shear strength during loading, as well as the evolution of the true contact area is difficult to estimate a priori. This issues will be the focal point of investigation of this thesis work.

To this end, discrete dislocation plasticity simulations (Van der Giessen and Needleman, 1995) are preformed for metal surfaces with simple geometry. Discrete dislocation plasticity is a numerical technique that has proven capable to capture and predict size dependent plasticity (Kreuzer and Pippan, 2007; Nicola et al., 2008, 2003, 2006; Sun et al., 2012; Widjaja et al., 2007). The analysis is performed on simplified surface geometries: asperities have either rectangular or sinusoidal shape. Conceivably, an improved understanding of the contact behavior of simple plastically deforming surfaces will pave the way to comprehend the contact and friction behavior of real surfaces.

1.2. Outline of the thesis

The thesis consists of a general introduction and four chapters, organized as follows:

In Chapter 2 the flattening of a single crystal with sinusoidal surface is studied by means of dislocation dynamics simulations. The amplitude and wavelength of the sinusoid is varied to investigate the effect of size and shape on the contact pressure required to flatten the surface to a given depth. Results show that smaller asperities are harder to flatten than large ones and that the contact pressure profile is characterized by very high peaks, in relation to the discontinuous nature of the contact area.

Chapter 3 focuses on interaction between neighboring sinusoidal asperities. Spacing between asperities is varied while the asperity size is kept constant. The simulations highlight an asperity density effect, i.e. the mean contact pressure necessary to flatten closely spaced asperities is found to be larger than that required to flatten widely spaced asperities. This asperity density effect is also observed for a purely elastic material, but it is enhanced for small asperities, in the presence of dislocation plasticity. Plastic strain gradients, dislocation limited plasticity and interaction between neighboring plastic zones all contribute to what we will call the asperity density effect.
In Chapter 4 and 5 flattening of the asperities is followed by shearing. In order to simplify the problem, and have a constant contact area, the shape of the asperities is changed from sinusoidal to rectangular.

In Chapter 4 a single asperity is sheared after flattening to different flattening depths. The results reveal 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. Multiple rectangular asperities are also sheared to investigate whether there is a similar asperity density effect as that observed for flattening in Chapter 3. An effect of asperity spacing is found 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.

Chapter 5 aims to investigate the dry frictional behavior of a rectangular asperity. Sliding of a contact point is taken to occur when the shear traction exceeds the normal traction at that point times a friction coefficient. Results show that at large contact pressures and friction coefficients, plasticity controls the frictional behavior of the single asperity.

References


References


Plastic flattening of a sinusoidal metal surface

The plastic flattening of a sinusoidal metal surface is studied by performing plane strain dislocation dynamics simulations. Plasticity arises from the collective motion of discrete dislocations of edge character. Their dynamics is incorporated through constitutive rules for nucleation, glide, pinning and annihilation. By analyzing surfaces with constant amplitude we found that the mean contact pressure is inversely proportional to the wavelength. For small wavelengths, due to interaction between plastic zones of neighboring contacts, the mean contact pressure can reach values that are about 1/10 of the theoretical strength of the material, thus significantly higher than what is predicted by simulations that do not account for size dependent plasticity. Surfaces with the same amplitude to period ratio have a size dependent response, such that if we interpret each period of the sinusoidal wave as the asperity of a rough surface, smaller asperities are harder to be flattened than large ones. The difference between the limiting situations of sticking and frictionless contacts is found to be negligible.

2.1. Introduction

Due to roughness, contact between two surfaces occurs primarily at the summits of the surface asperities, so that the area really affected by contact is just a small fraction of the body surface. Nevertheless, the forces generated in such a small area are responsible for most tribological phenomena, like friction and wear.

In general the surface topography is a mixture of shapes spanning different length scales and can nowadays be measured with high precision. By contrast, the change in contact area during loading is not easily measurable. Since the contact area evolves in a non-trivial way during contact, knowledge of the initial topography is of little use for determination of friction during contact (Zhang et al., 2010). Therefore, rough surface modeling can contribute to the prediction of friction by allowing to track the evolution of the area of contact as well as the contact pressure during loading.

Traditional contact mechanics models based on the work of Greenwood and Williamson (Greenwood and Williamson, 1966) give an approximate evaluation of contact area and pressure for a collection of asperities, but they neglect the elastic interaction between asperities. More precise predictions can be obtained using the statistical friction models, like Persson’s (Persson, 2001) and its modification by Müser (Müser, 2008), but these works mainly focus on the assumption that the flattened asperities behave elastically. The pressure predicted by such models exceeds the hardness of the material on many contacts at rather low loads. In addition to that, experimental studies of rough surface contact (Dieterich and Kilgore, 1996; Dwyer-Joyce et al., 2001) indicate that the pressure in the contacts is sufficiently high for plastic deformation to take place. We therefore believe it is of interest to investigate what role plasticity really plays. Even though it might be expected that the change in contact area and pressure would depend strongly on the plastic deformation of the asperities, finite element simulations of elasto-plastic bodies with a rough surface by Pei et al. (Pei et al., 2005) seem to disprove that, and to indicate that when the material behaves plastically, self-affine surfaces with different morphology deform in a similar way. Their results also confirm the interesting finding by Gao et al. (Gao and Bower, 2006) that the mean contact pressure of each asperity of the surface is increased by interaction between neighboring asperities but limited to approximately twice the single asperity hardness. Gao et al. (Gao and Bower, 2006) account for the elastic-plastic interaction of neighboring asperities and find that this interaction hinders flattening of the surface, to the point that the true contact area converges to zero.
The purpose of this publication is to shed some light on the role of size dependent plasticity in the flattening of a rough metal surface. The roughness of the surface is strongly simplified to a sinusoidal wave function, but plasticity caused by dislocation glide is carefully computed by discrete dislocation simulations (Van der Giessen and Needleman, 1995). The numerical technique has so far proven successful to capture size dependent plastic behaviour of isolated flat contacts (Deshpande et al., 2004) as well as interplay between plasticity underneath arrays of flat contacts (Nicola et al., 2007, 2008).

2.2. Formulation

The model problem is shown in Fig. 2.1. A rigid platen flattens the sinusoidal surface of a semi-infinite single crystal with amplitude $A$ and wavelength $w$. The top surface of the crystal is described by

$$f(x_1) = h - A \cos\left(\frac{2\pi x_1}{w}\right).$$

The analysis is performed on a unit cell encompassing a full period of the surface wave and periodic boundary conditions are imposed at the right and left borders of that cell. The load is imposed by prescribing the vertical displacement of the rigid platen:

$$u_2(x_1, f(x_1)) = -\int \dot{u} dt, \quad x_1 \in \mathcal{C},$$

(2.1)
where \( C \) is the contact area, defined as the flat region of intimate contact between the flat platen and the crystal where displacement is prescribed. By regions of intimate (or true) contact we refer to sum of areas where two or more adjacent surface nodes are in contact with the platen. Outside the contact region, the top surface \( (x_2 = f(x_1)) \) is traction free. The traction distribution along the contact normal to the platen determines the flattening force \( F_n \) (per unit of length):

\[
F_n := - \int_{x_1 \in C} \sigma_{22} dx_1.
\]  

(2.2)

Imposing boundary conditions that account for realistic interaction between surface and platen is compromised by the lack of knowledge about the friction coefficient between surfaces at such scale. Therefore we confine our study to the two limiting situations for the contact conditions:

frictionless (non adhesive) contact: \( \sigma_{12}(x_1, f(x_1)) = 0, \quad x_1 \in C, \)  

(2.3)

sticking (adhesive) contact: \( u_1(x_1, f(x_1)) = 0, \quad x_1 \in C. \)  

(2.4)

Periodic boundary conditions are imposed at the vertical sides of the unit cell,

\[
u_1 (w, x_2) - u_1 (0, x_2) = U_1, \quad u_2 (0, x_2) = u_2 (w, x_2).
\]  

(2.5)

For crystals with sticking contacts the value of the uniform expansion \( U_1 \) is taken to be zero. This condition is necessary to fulfil the requirements that (1) the platen must be rigid and (2) the contacts stick to the platen. Note that even if the unit cell is bound to not expand, i.e. \( U_1 = 0 \), the lateral boundaries of the unit cell are not constrained to remain straight. For the frictionless contacts we will consider two possibilities: \( U_1 = 0 \) or \( U_1 \) is determined from the condition that lateral expansion of the unit cell can take place freely, since the material can slide underneath the contacts, as expressed by

\[
\Sigma_{11} := \frac{1}{h} \int_0^{h-A} \sigma_{11}(x_1, x_2) dx_2 = 0.
\]  

(2.6)

We will therefore analyze three different boundary value problems, that will be referred to as follows:

- Sticking-Constrained (S-C): no slip at the contacts, Eq. (2.4), and no overall lateral strain, i.e. \( U_1 = 0 \);

- Frictionless-Constrained (F-C): no friction at the contact, Eq. (2.3), and no...
2.2. Formulation

overall strain, \( U_1 = 0 \);

- Frictionless-Unconstrained (F-U): no friction at the contact and no overall stress \( \Sigma_{11} = 0 \) (free expansion of the unit cell), Eq. (2.6).

A comparison between results obtained with the first two boundary conditions, S-C and F-C, will give insight in the importance of the friction conditions at the contact. Contrasting the last two conditions, F-C and F-U, will instead tell us if the material that can slide underneath the contact will behave differently if given the possibility to expand. For further reference the boundary conditions studied are summarized in Table 2.1.

Table 2.1: Contact conditions and conditions on the horizontal expansion \( U_1 \) of the unit cell.

<table>
<thead>
<tr>
<th>Contact-Expansion</th>
<th>Contact conditions</th>
<th>Expansion conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>S-C</td>
<td>Eq. (2.4)</td>
<td>Eq. (2.5); ( U_1 = 0, \Sigma_{11} \neq 0 )</td>
</tr>
<tr>
<td>F-C</td>
<td>Eq. (2.3)</td>
<td>Eq. (2.5); ( U_1 = 0, \Sigma_{11} \neq 0 )</td>
</tr>
<tr>
<td>F-U</td>
<td>Eq. (2.3)</td>
<td>Eq. (2.6); ( U_1 \neq 0, \Sigma_{11} = 0 )</td>
</tr>
</tbody>
</table>

The simulations follow the formulation for discrete dislocation plasticity by Van der Giessen and Needleman (Van der Giessen and Needleman, 1995): the solution for the dislocated crystal is given by the linear composition of the closed-form elastic solution for the dislocations in an infinite medium and the numerical correction for the image fields. The latter is calculated by the finite element method. The mesh is made of very fine square elements at the surface of the crystal, to correctly capture the contact area and the dislocation fields, the mesh is coarser at the bottom of the crystal, where there are no dislocations.

The crystal is taken to have the elastic properties of aluminum: Young’s modulus \( E = 70 \) GPa and a Poisson’s ratio \( \nu = 0.33 \). Following Rice (Rice, 1987) the FCC crystal is modeled in two dimensions by considering three potentially active slip systems with orientations \( \varphi = 0^\circ, 60^\circ \) and \( 120^\circ \). The spacing between slip planes in the crystal is \( 200b \), where \( b \) is the Burgers vector of magnitude \( b = 0.25 \) nm. At the beginning of the simulation, the crystal is dislocation free and it contains a given density of obstacles and dislocation sources distributed randomly on the slip planes in the crystal. The obstacles represent small precipitates in the material as well as forest dislocations present as a consequence of previous plastic deformation. When the resolved shear stress at the dislocation sources is sufficiently high, edge dislocations are generated. The mean nucleation strength for
the sources is taken to be $\tau_{nuc} = 50$ MPa, with 20% standard deviation. The time span necessary for nucleation of a dislocation dipole, $t_{nuc}$, is taken to be 10 ns. The values used in these simulations are the outcome of a quantitative comparison with experimental results in (Nicola et al., 2006).

### 2.3. Effect of boundary conditions

Two crystals with average height $h = 12 \, \mu m$ and surface amplitudes $A = 0.2 \, \mu m$ and $A = 0.8 \, \mu m$ are flattened by $u = 0.04 \, \mu m$. The spacing between contacts $w$, which corresponds also to the width of the unit cell, is taken to be constant and initially rather wide, i.e. $w = 10 \, \mu m$. The density of dislocation sources and obstacles is $\rho = 30 \, \mu m^{-2}$. The simulations are performed using the three different combinations of boundary conditions defined in Table 2.1: sticking-constrained (S-C), frictionless-constrained (F-C) and frictionless-unconstrained (F-U). The flattening force and the corresponding true contact area during flattening are compared in Fig. 2.2a and b, respectively. The curves for sticking (S-C) and frictionless (F-C) contacts are very close to each other. A larger difference emerges between constrained (F-C) and unconstrained (F-U) crystals. From this observation we conclude that the nature of the contact itself, be it frictionless or sticking, does not affect the flattening of the surface. Instead, flattening is affected by the extent to which the material is free to expand laterally underneath the contacts.

![Figure 2.2: (a) Force versus depth and (b) contact area evolution for S-C, F-U and F-C crystals for $A = 0.2$ and $0.8 \, \mu m$. Each curve represents the average of different realizations, i.e. different initial distributions of sources and obstacles strengths and locations.](image-url)
or constrained to maintain the same width in between contacts. The influence of lateral boundary conditions (constrained or unconstrained) does not depend on surface amplitude. At a flattening depth of 0.04 \( \mu \text{m} \) for \( A = 0.2 \mu \text{m} \) the measured force for unconstrained crystals is 15\% smaller than that for constrained crystals, their contact area is 9\% smaller. For \( A = 0.8 \mu \text{m} \), the difference in force is 17\% and the difference in contact area is 8\%.

![Figure 2.3: The distribution of horizontal displacement \( u_x \) for the crystal with amplitude \( A = 0.2 \mu \text{m} \) under (a) S-C, (b) F-C and (c) F-U contacts at the depth of 0.04 \( \mu \text{m} \).](image)

For the crystal with smaller amplitude, we choose a representative realization.
and show the distribution of the displacements in $x_1$-direction together with the dislocations at final depth (in Fig. 2.3). The figure confirms that the flattening under frictionless contacts occurs partly by lateral expansion of the material. Also, the figure gives further evidence that the difference in contact conditions is not significant, cf. Fig. 2.3a vs 2.3b, but that only the possibility of expansion affects the deformation mode, Fig. 2.3c. The distribution of displacement in $x_2$ direction

Figure 2.4: The distribution of vertical displacement $u_2$ for the crystal with amplitude $A = 0.2 \ \mu$m at the depth of $0.04 \ \mu$m for various boundary conditions: (a) S-C (b) F-C and (c) F-U.

for the same crystals is shown in Fig. 2.4. It is clearly seen in this figure, that material in the crystal with constrained boundary conditions (S-C and F-C) piles up
in the vicinity of the contact areas (see Fig. 2.4a and b), whereas pile-up does not occur in the F-U crystal (Fig. 2.4c) due to lateral expansion.

![Figure 2.5: Surface profile in the contact region for constrained and unconstrained crystals at the flattening depths of 0.02 μm and 0.04 μm for amplitudes (a) A = 0.2 μm and (b) A = 0.8 μm. Black segments indicate the areas of true contact with the platen.](image)

It is important to note that even though the virgin surface is smooth and the platen is rigid, the surface does not remain smooth. This is illustrated by the surface profiles in Fig. 2.5 at flattening depths $u = 0.02$ μm and $0.04$ μm. We observe that the contact area for all amplitudes and contact conditions evolves in a discontinuous way during flattening. This behavior is caused by the steps that are left when dislocations glide out of the free surface. The protruding parts of those displacement steps can create new contact with the rigid platen, while other parts will remain untouched. Therefore, the true contact area is the sum of distinct patches of contact and is significantly smaller than the apparent contact area would be (if measured from the first contacting point to the last one). The exit of dislocations is a stochastic process, so that different realizations show a different local evolution of the true contact area. The observation (cf. From Fig. 2.5a and Fig. 2.2b) that the contact area for the constrained crystal is slightly larger than that for the unconstrained crystal is not specific for the realization shown in Fig. 2.5 but is characteristic of all six realizations studied. The larger contact area in constrained crystals can be attributed to the presence of material pile ups, see Fig. 2.4a and b, that help the formation of new contact regions.
Plastic flattening of a sinusoidal metal surface

Figure 2.6: Flattening force versus depth for crystals with period \( w = 2.5 \ \mu m \) with unit cell of size \( W = 2w, 2w \) and \( 3w \). The labels #1 and #2 indicate realizations with different locations of dislocation sources.

The simulations reported on so far are for unit cells that encompass only a single wave of surface. When the unit cell width is small, the statistical variation of dislocation and sources locations is also small. To explore the effect of a larger source sampling, simulations are performed for unit cells of width \( W \) containing two or three wave periods \( w \). The corresponding pressure-displacement curves in Fig. 2.6 show that the mean contact pressure is not affected: the difference between these curves is smaller than the difference between curves obtained by simulations with identical unit cells but with a different location of dislocation sources (indicated in the figure by #1 and #2). Therefore in the rest of the paper we will perform simulations only for \( W = w \).

2.4. Effect of surface shape \( A/w \)

Flattening the sinusoidal surface of a single crystal is a problem that involves several lengths: the period \( w \) and amplitude \( A \) of the surface, the height of the crystal \( h \) and the average spacing between dislocation sources \( L_{ave} = 1/\sqrt{\rho_{nuc}} \). If the source density is large enough to ensure that sufficiently many dislocations are nucleated when needed, the source spacing \( L_{ave} \) will not affect the results and the behavior will depend only on \( w, A \) and \( h \).

We here investigate the effect of changing period \( w \) on surface pressure while keeping the other lengths constant: \( A = 0.3 \ \mu m, h = 12 \ \mu m \) and \( L_{ave} = 0.18 \ \mu m \). We will confine attention to crystals with frictionless contacts and constrained
2.4. Effect of surface shape $A/w$

Figure 2.7: (a) Mean contact pressure as a function of flattening depth for different periods $w$ and constant amplitude $A = 0.3 \, \mu m$. The dashed curves indicate the elastic solutions. (b) Normalized mean contact pressure versus $\varepsilon_d$ for various periods $w$ and two different crystal heights.

unit cells. Figure 2.7a shows how the mean contact pressure,

$$P_m = \frac{1}{C} \int_{x_1 \in C} \sigma_{22} \, dx_1,$$

(2.7)

where $C$ is the true contact area, increases with decreasing period for surfaces with $w = 1.875, 2.5, 3.75, 7.5$ and $15 \, \mu m$. This trend is expected and in agreement with the elastic behaviour of the crystal, since the contact fraction, $C/w$, increases with increasing period. Anyhow, since our goal is to study the behavior of the surface and not of the whole crystal under flattening, we plot in Fig. 2.7b the mean contact pressure $P_m$, normalized by $AE^*/w$, as a function of the flattening strain $\varepsilon_d = (d_0 - d)/d_0$ (note that this parameter is similar to that introduced by Persson (Persson, 2007)), but differs in the normalization distance $d_0$ rather than the $rms$ of the original surface). Here, $d$ is the separation distance between the platen and the average height of the crystal surface, $d_0$ the initial separation distance and $E^* = E/(1 - \nu^2) \approx 78.5$ GPa. Normalizing the pressure by $AE^*/w$ allows us to obtain elastic curves that are almost overlapping, by that facilitating comparison between surfaces with different $w$. Also, these curves do not contain any dependence on the crystal height $h$, as shown in Fig. 2.7b by comparing results for crystals with $h = 12 \, \mu m$ and $h = 24 \, \mu m$. By looking at Fig. 2.8a we can see that the plastic response of the surfaces of crystals with various $w$ are very close to each other, deviation from elasticity occurring at about $\varepsilon_S = 0.007$. 
If we want to approach the limit of continuum plasticity we can repeat the simulations in Fig. 2.7 with a higher density of dislocation sources. We observed that decreasing the spacing between dislocation sources below $L_{ave} = 0.13 \mu m$ does not affect the results; for $L_{ave} = 0.13 \mu m$ we obtain curves that are almost overlapping (see Fig. 2.8a). The plastic response of the surface does not additionally depend on $w$, i.e. $P_m$ is just inversely proportional to $w$, meaning that plasticity in the asperities is size independent. For a twice as large dislocation source spacing, though, i.e. four times as large dislocation density, results are significantly different and reveal a clear size dependence: surfaces with smaller $w$ are harder than surfaces with a larger $w$ (see Fig. 2.8b). Thus, if $w/L_{ave} < 3.75/0.26 \approx 15$ and for a constant $A$, the onset of plasticity is still inversely proportional to $w$ but plastic curves have considerably different strain hardening. For a better look at what happens locally for different wavelengths $w$, Fig. 2.9a and b show the stress state and the dislocation structures for $w = 15$ and $2.5 \mu m$ for the smallest source spacing, $L_{ave} = 0.13 \mu m$. Note that the stress level of the lower part of the two crystals is different because the nominal pressure differs by a factor six (cf. Fig. 2.8a). The state in the subsurface regions is very different, with the crystals with smaller period having a very high density of dislocations everywhere in the top $\sim 2 \mu m$ of the crystal. By contrast, there is an isolated plastic zone underneath the contact in the crystal with larger period. This translates into the dislocation density being higher for the smaller $w$, see Fig. 2.9c, for both source densities tested. The fact
that the dislocation density increases with decreasing period, together with the dislocation distribution in Fig. 2.9b, indicates that the plastic zones underneath neighboring asperities interact progressively more as the period is decreased, thus giving rise to progressively larger mean contact pressures. Our expectation is that these results will still be valid in the case of a microcrystalline material, based on the following considerations: (a) if the grain size is much larger than the contact spacing most grain boundaries will be located outside of the plastic zones and therefore not affect the results; (b) if the grain size is comparable to contact spacings, the grain boundaries that are in the plastic zone will affect it by hindering dislocation motion. The hindering of dislocation glide has two opposite effects on contact pressure: on the one hand it decreases it by reducing the interaction
between plastic zones, on the other hand it enhances contact pressure because plasticity in the crystal is reduced.

![Diagram](image)

Figure 2.10: Contact pressure distribution for surfaces with different periods at \( \varepsilon_d = 0.056 \) when the source spacing is (a) \( L_{ave} = 0.13 \mu m \) and (b) \( L_{ave} = 0.26 \mu m \).

The detailed pressure distribution on the contacts is given in Fig. 2.10. Surfaces with larger periods make discontinuous contact with the flat platen (see also Fig. 2.5), while surfaces with smaller periods are characterized by a single contact region. As a consequence of the fact that the contact area is patchy, the distribution of contact pressure on surfaces with larger roughness periods is highly nonuniform: the larger region of contact has a much lower average stress than the smaller contact patches around it, which are subjected to very high stress peaks (see Fig. 2.10). The average mean contact pressure found on each asperity for \( w = 15 \mu m \) is about \( 6\sigma_y \) \(^1\) for the large source density and about \( 7\sigma_y \) for the low source density. For \( w = 2.5 \mu m \) the mean contact pressure is remarkably higher, i.e. \( P_m \approx 38\sigma_y \) for the large source density and \( P_m \approx 56\sigma_y \) for small source density. These findings are in contrast with what is predicted by classical plasticity simulations (Gao et al., 2006; Pei et al., 2005), according to which contacts are continuous and the mean contact pressure on a single asperity is limited to about \( 6\sigma_y \). While the discontinuous nature of contact in our simulations and the corresponding high stress concentrations can be unrealistically high due to the fact that the simulations are two dimensional, surface steps due to plastic activity are real so that patchy contact is likely to occur in reality.

\(^1\) \( \sigma_y \approx 50 \) MPa for a single crystal with the same material properties as those of the crystals here considered under uniform compression.
So far we have varied the surface shape \( A/w \) by changing \( w \) and keeping \( A \) constant. Next, we carry out simulations for various amplitudes of the sinusoidal wave i.e. \( A = 0.2, 0.4, 0.6 \) and \( 0.8 \) \( \mu \text{m} \), by keeping the period fixed at \( w = 10 \) \( \mu \text{m} \).

![Figure 2.11](image-url)

Figure 2.11: (a) Normalized mean contact pressure as a function of \( \varepsilon_d \) for varying amplitudes on crystals with \( L_{ave} = 0.26 \) \( \mu \text{m} \) or \( L_{ave} = 0.13 \) \( \mu \text{m} \). (b) Yield pressure for surfaces with various amplitudes and constant period, \( w = 10 \mu\text{m} \) (black symbols) and with various periods but constant amplitude, \( A = 0.3 \) \( \mu \text{m} \) (red symbols). Results are reported for small and large source spacing, and each data point is the average over six realizations. Lines are linear fits through the data points for the same source densities.

Figure 2.11a shows the mean contact pressure normalized by \( (AE^*/w) \) as a function of \( \varepsilon_d \) for various source spacings. Just as for the previous simulations, the elastic solutions overlap, but the onset of plasticity depends on amplitude. Increasing the average spacing between sources from \( L_{ave} = 0.13 \) \( \mu \text{m} \) to \( 0.26 \) \( \mu \text{m} \), i.e. decreasing the source density, results in a further increase of the relative difference in the onset of plasticity.

In order to clarify how the onset of yield depends on amplitude at constant period and on period at constant amplitude, we here define the yield pressure \( P_{my} \) as the intersection between the \( P_{m}w/AE^* \) versus \( \varepsilon_d \) curve and the corresponding elastic curve offset by \( \varepsilon_S = 0.2\% \) (in the same spirit as the usual definition of the 0.2% yield stress in macroscopic plasticity). All the results for yield pressure obtained in this and the previous section have been compiled in Fig. 2.11b as a function of \( A/w \). As previously noticed, the yield pressure at constant amplitude is inversely proportional to period, but we now also observe that the constant of proportionality increases with the source spacing. Even though we know from Fig. 2.11a that the surface yield pressure is not proportional to amplitude, i.e. the...
deviation from the elastic curve does not occur at the same $P_m w/AE^*$, the yield values extracted from Fig. 2.11a, as shown in black in 11b, vary linearly with $A/w$ with a slope $0.087E^*$. If the source density is decreased the surface becomes harder, but the constant of proportionality does not change. The interesting observation in this figure thus is that if we compare surfaces with the same $A/w$, i.e. with the same root mean square slope, $h_{rms} = \sqrt{2} \pi A/w$, the yield pressure $P_{m_y}$ is not unique, but depends on the specific choice of $w$ and $A$. This signifies a size effect which we will investigate in more detail in the coming section.

2.5. Size dependence at constant shape $A/w$

In this section we compare the behavior of surfaces that have the same amplitude-to-period ratio $A/w$, but have various values for $A$ and $w$. Specifically, we perform simulations for waves with $A/w=0.02$ with periods $w=2.5, 5, 10$ and $15 \mu m$ and for $A/w=0.05$, with periods $w=2.5, 6, 8$ and $10 \mu m$.

![Figure 2.12](image)

Figure 2.12: (a) Mean contact pressure normalized by $AE^*/w$ and (b) residual dislocation density versus $\varepsilon_d$ for amplitude-to-period ratios 0.02 and 0.05, with source spacing $L_{ave} = 0.13 \mu m$.

Figure 2.12a shows the mean contact pressure as a function of $\varepsilon_d$. The blue dashed line represents the corresponding elastic solution. If we interpret each period of the sinusoidal wave as the asperity of a rough surface, the results show that the plastic deformation of asperities is size dependent: for a given amplitude-to-period ratio, the pressure required to flatten a smaller asperity is larger than for a larger asperity. The larger mean contact pressure for the smaller asperity is partly due to fewer dislocations being nucleated in the crystal as shown in Fig. 2.12b. In
order to get further insight in the origin of this, Figures 2.13 show the stress distribution and dislocation structure inside crystals with $A/w = 0.05$ at $\varepsilon_d = 0.056$. The plastic zone increases with increasing asperity size (i.e. increasing amplitude $A$ and period $w$). At the same time, the dislocation density also increases (see Fig. 2.12b). The size dependence seems therefore to be caused by limited availability of dislocations underneath the smaller contact areas, which indeed is seen in Fig. 2.13.

### 2.6. Conclusions

Two dimensional simulations are performed to investigate the flattening of a sinusoidal surface with the discrete dislocation plasticity method. Three limiting situations have been considered: the contacts are perfectly sticking (S-C), frictionless (F-U), frictionless but constrained to not expand laterally (F-C). Results have shown that:

- for sinusoidal surfaces of any period and amplitude, the contact conditions, i.e. frictionless or sticking, do not affect the flattening force nor the mean contact pressure during flattening;

- on the contrary, results depend on whether or not the material is free to expand laterally underneath the contacts. Such dependence is not affected by surface shape. If the material is constrained (which is a more reasonable assumption if we consider the constraint that the crystal would be subjected to from the material in the in-plane direction):

---

**Figure 2.13:** Stress distribution $\sigma_{22}$ for F-C crystals with constant ratio $A/w = 0.05$ at $\varepsilon_d$ for different wavelengths (a) $w = 2.5 \, \mu m$, (b) $w = 6 \, \mu m$, (c) $w = 8 \, \mu m$ and (d) $w = 10 \, \mu m$. 


Plastic flattening of a sinusoidal metal surface

- a larger force is needed to flatten the surface to a given depth;
- a larger contact with the flattening body is achieved;
- material pile up appears in the free surface region close to the contact.

By analyzing surfaces with various $A/w$ we found that,

- for surfaces with constant amplitude

  - the mean contact pressure increases with decreasing period. The mean contact pressure can reach values up to about $40\sigma_y$, thus significantly higher than what is predicted by simulations that do not account for size dependent plasticity (Gao et al., 2006).
  - the mean contact pressure is inversely proportional to period at any strain as long as the source spacing is small enough;
  - a threshold period-to-average source spacing of about 15 is found, below which it becomes even more difficult to flatten the sinusoidal surface due to additional strain hardening caused by limited source availability underneath the contacts and by plastic interaction of the asperities;
  - the yield pressure $P_{my}$ is inversely proportional to period for all source spacings tested; the constant of proportionality is larger for larger source spacings.

- for surfaces with constant period:

  - the yield pressure can be approximated as being proportional to amplitude. The same proportionality constant $0.087E^*$ holds for small and large source spacings.

- A size dependent response is found for crystals with surfaces with the same amplitude-to-period ratio, with smaller asperities being more difficult to be deformed plastically to the same strain. As a consequence, the curves that describe the relation between load and contact area and between load and separation distance are non unique for a given $A/w$, but depend on the specific choice of $A, w$.

- As a consequence of the fact that the area of intimate contact is discontinuous, the distribution of contact pressure is highly non homogeneous: the larger region of contact underneath the asperity has a much lower average
stress than the smaller contact regions around it, which are characterized by a very high stress concentration.

It is noteworthy that these results aim at underlying the importance of size dependent plasticity in contact mechanics but cannot straightforwardly be extended to the plastic contact between two rough surfaces. When two rough surfaces are brought into contact and plastically deform, the behavior is generally more complex than in the case of a rough surface flattened by a platen. Size dependent behavior of the asperities on both surfaces complicates matters even further.

References


Interaction between neighboring asperities during flattening

Discrete dislocation plasticity simulations are performed to investigate the role of interaction between neighboring asperities on the contact pressure induced by a rigid platen on a rough surface. The rough surface is modeled as an array of equispaced asperities with a sinusoidal profile. The spacing between asperities is varied and the contact pressure necessary to flatten the surface to a given strain is computed. Plasticity in the asperities and in the crystal below is described by the collective glide of dislocations of edge character.

Results show that the mean contact pressure necessary to flatten closely spaced asperities is larger than that required to flatten widely separated asperities. A small dependence on asperity density is already observed for a purely elastic material, but it is enhanced for small asperities, in the presence of dislocation plasticity. Plastic strain gradients, dislocation limited plasticity and interaction between neighboring plastic zones all contribute to what we will call the asperity density effect. Since dislocation limited plasticity plays a

dominant role, the asperity density effect will mainly be relevant for surfaces having small asperity roughness.
3.1. Introduction

Friction and wear arise when two rough surfaces are brought into contact and then sheared with respect to each other. If the contacting bodies are made of metal, their surfaces are inevitably rough after production and contain asperities spanning various length scales that deform during loading. Deformation of the asperities is not only crucial in determining the size of the contact at a given load but also in controlling friction. When the asperities are pressed against each other, high stresses develop locally and plastic deformation of asperities is unavoidable. Several experimental studies (Dieterich and Kilgore, 1996; Dwyer-Joyce et al., 2001) indeed report that the pressure measured at the contacts is sufficiently high for plastic deformation to take place. Also state-of-the-art statistical friction models, like those of Persson (Persson, 2001) and Müser (Müser, 2008), predict contact pressures that exceed the hardness of the material on several contact areas at rather low applied loads.

This raises important issues since there is a large body of evidence that both the indentation hardness of the material (Kreuzer and Pippan, 2007; Pharr et al., 2010; Widjaja et al., 2007; Zong and Soboyejo, 2005) and the yield strength in tension (Greer et al., 2005; Nicola et al., 2003; Volkert and Lilleodden, 2006) are size dependent quantities: they are not material constants but depend on the size of the plastically deforming material. Hence, what is the hardness that the material should reach for plasticity to take place? Attention so far has mainly focused on size-dependent plasticity in simple small objects like pillars and thin films, but given that metal roughness is a mixture of asperity shapes spanning various length scales, it has to be expected that size dependent plasticity may play a pivotal role.

In relation to this it is possible to address a long-standing problem related to surface plasticity, namely the persistence of roughness under contact loading. By ‘persistence’ we refer to the capability of the surface asperities to withstand pressures larger than the material hardness, interpreted through the Tabor relationship as $\sim 3$ times the macroscopic yield strength. Persistence was shown experimentally by Childs (Childs, 1977) already in 1977 and attributed to interaction between plastic zones underneath asperities. More recently, Gao and coworkers (Gao et al., 2006) performed continuum plasticity simulations of the flattening of sinusoidal asperities and found that, in order for the sinusoidal surface to be plastically flattened, the applied pressure needed to be twice the material hardness. In view of the multi-scale nature of surface roughness, Gao and Bower (Gao and Bower, 2006) performed similar simulations on a fractal surface with a Weierstrass profile and found out that the surface could actually never be flattened.
These studies, though, have the limitation that they assume that continuum plasticity be applicable at all scales whereas it is well known now that plasticity is size dependent below tens of micrometers. We will here use Discrete Dislocation plasticity (DD), which is a numerical technique that describes plastic deformation by accounting for the collective glide of discrete dislocations. By virtue of the characteristic length it contains, this method has proven successful in capturing the size dependent behavior of micron-scale metal crystals under various loading conditions (Kreuzer and Pippan, 2007; Nicola et al., 2008, 2003, 2006; Sun et al., 2012; Widjaja et al., 2007). In a recent study (Sun et al., 2012) we have analyzed the contact between a rigid platen and plastically deforming body with sinusoidal profile, where each period of the wave was interpreted as the asperity of a rough surface. A size effect was found for decreasing asperity size, with smaller asperities being harder to flatten than larger ones. One limitation of our previous study was that, by considering a sinusoidal surface we could not identify the effect of the spacing between asperities on plastic deformation separately: closely spaced asperities in a sinusoidal wave are also smaller asperities.

Building on the above-mentioned study, the surface of the metal crystal is here taken to be an array of equispaced asperities of sinusoidal shape. In this way the spacing between asperities can be independently changed while keeping the size and shape of each individual asperity constant. The main purpose of the present paper is to investigate whether there is an effect of asperity density—in other words, the spacing between asperities—and what are the origins of this effect.

### 3.2. Formulation

#### 3.2.1. Boundary value problem

A rigid body flattens the surface of a metal single crystal as shown schematically in Fig 3.1. The surface is characterized by an array of equally spaced asperities that have a sinusoidal profile with wavelength \( w \) and amplitude \( A \). The spacing between asperities is \( s \). Periodic boundary conditions are imposed at the right and left borders of the unit cell of width \( s \). The load is applied by prescribing the vertical displacement of the rigid platen over the current contact area \( C \):

\[
 u_2(x_1, f(x_1)) = - \int \dot{u} dt, \quad x_1 \in C. \tag{3.1}
\]
3.2. Formulation

Figure 3.1: Two-dimensional model of a single crystal with sinusoidal surface asperities flattened by a rigid platen.

Here, the top surface of the crystal is described by,

\[
 f(x_1) = \begin{cases} 
 h - A \cos \left( \frac{2\pi x_1}{w} \right), & x_1 \in (0, w] \\
 h - A, & x_1 \in (w, s], 
\end{cases} 
\]  

(3.2)

where \( h \) is the height from the bottom of the crystal to the mean height of the asperity. The contact area \( C \) is defined as the flat region of intimate contact between the flat platen and the crystal. Outside the contact region, the top surface is traction free. The traction distribution along the contact normal to the platen determines the flattening force \( F \) (per unit of length):

\[
 F := - \int_{x_1 \in C} \sigma_{22} dx_1. 
\]  

(3.3)

Imposing boundary conditions that account for a realistic interaction between surface and platen is very challenging, since the friction coefficient between surfaces at such scale is unknown. In our previous study (Sun et al., 2012), we analysed the effect of frictionless and sticking contacts and we found a negligible difference in the plastic response of the surface. Therefore this study is confined to the limiting situation of frictionless contacts:

\[
 \sigma_{12}(x_1, f(x_1)) = 0, \quad x_1 \in C. 
\]  

(3.4)

Periodic boundary conditions are imposed at the vertical sides of the unit cell,

\[
 u_1 (0, x_2) = u_1 (s, x_2), \quad u_2 (0, x_2) = u_2 (s, x_2). 
\]  

(3.5)
Even though the lateral expansion of the unit cell is taken to be zero, the lateral boundaries of the unit cell are not constrained to remain straight but can fluctuate about $x_1 = 0$ and $x_1 = s$. Additional boundary conditions are prescribed at the bottom of the crystal:

$$u_2 (x_1,0) = 0, \quad u_1 (0,0) = 0. \quad (3.6)$$

### 3.2.2. Discrete dislocation plasticity

The simulations follow the formulation for discrete dislocation (DD) plasticity by Van der Giessen and Needleman (Van der Giessen and Needleman, 1995): the solution for the dislocated crystal is given by the linear superposition of the closed-form elastic solution for the dislocations in an infinite medium and the numerical correction for the boundary conditions. The latter is calculated by the finite element method. The stress state in the body governs the evolution of the dislocation structure by a series of constitutive rules, which are similar to those proposed in (Nicola et al., 2007) and (Nicola et al., 2008). Nucleation, glide, annihilation of dislocations, as well as pinning at obstacles are controlled by these rules.

At the beginning of the simulation, the crystal is dislocation free and it contains a given density of obstacles and Frank-Read sources distributed randomly on the slip planes in the crystal. Nucleation occurs by activation of Frank-Read sources. Once the shear stress acting on a source is larger than its critical strength, $\tau_{nuc}$, for a time span $t_{nuc}$ a new dislocation loop forms. In two dimensions, the dislocation loop is represented by a dipole of dislocations of edge character. The glide velocity $v^l$ of the $I$th dislocation is proportional to the Peach-Koehler force $f^l$, according to $v^l = f^l / B$ where $B$ is the drag coefficient. The obstacles represent small precipitates in the material as well as forest dislocations present as a consequence of previous plastic deformation. Dislocations can be pinned by the presence of point obstacles on the slip planes, each characterized by a critical strength, $\tau_{obs}$. As long as the Peach-Koehler force acting on the pinned dislocation is lower than the obstacle strength, the dislocation will be pinned at the obstacle, otherwise it will be released and continue to glide. Dislocations can freely leave the crystal through the top surface except where it is in contact with the platen; it is assumed that the contact interface is completely impenetrable for dislocations.

The crystal is taken to have the elastic properties of aluminum: Young’s modulus $E = 70$ GPa and a Poisson’s ratio $\nu = 0.33$. Following Rice (Rice, 1987) the FCC crystal is modeled in two dimensions by considering three potentially active slip systems with orientations $\varphi = 0^\circ$, $60^\circ$ and $-60^\circ$. The spacing between slip
planes in the crystal is 200\(b\), where \(b\) is the Burgers vector of magnitude \(b = 0.25\) nm. The mean nucleation strength for the sources is taken to be \(\tau_{\text{nuc}} = 50\) MPa, has a 20\% standard deviation and the obstacle strength is \(\tau_{\text{obs}} = 150\) MPa. The average source spacing \(L_{\text{nuc}}\) is 0.26 \(\mu m\), while the average obstacle spacing \(L_{\text{obs}}\) is 0.18 \(\mu m\), unless otherwise stated. The time span necessary for nucleation of a dislocation dipole, \(t_{\text{nuc}}\), is taken to be 10 ns. The values used in these simulations are the outcome of a quantitative calibration to experimental results in (Nicola et al., 2006).

### 3.2.3. Crystal plasticity

The DD results are here also compared to crystal plasticity (CP), of the type proposed by Pierce et al. (Peirce et al., 1983). The total strain rate is written as the sum of an elastic part and a viscoplastic part

\[
\dot{\varepsilon}_{ij} = \dot{\varepsilon}^e_{ij} + \dot{\varepsilon}^p_{ij}.
\]

The plastic part has the form

\[
\dot{\varepsilon}^p_{ij} = \sum_{\alpha} \dot{\gamma}_{\alpha} \mu_{\alpha}^i j,
\]

where \(\mu_{\alpha}^i j\) is the component of the slip plane normal and the slip direction of slip system \(\alpha\). The slip rate \(\dot{\gamma}_{\alpha}\) is taken to follow the viscoplastic power law

\[
\dot{\gamma}_{\alpha} = \dot{\gamma}_0 \frac{\tau_{\alpha}^{m-1}}{g_{\alpha}} \left(\frac{\tau_{\alpha}}{g_{\alpha}}\right)^{m-1},
\]

in terms of the resolved shear stress \(\tau_{\alpha} = m_{\alpha}^i j \sigma_{i j}^f\) on slip system \(\alpha\). Here, \(\dot{\gamma}_0\) is a reference slip rate, \(m\) is the strain rate sensitivity exponent and \(g_{\alpha}\) is the hardness of slip system \(\alpha\). It has an initial value \(\tau_0\) for all \(\alpha\) and evolves according to

\[
\dot{g}_{\alpha} = h_{\alpha \beta} \sum_{\alpha} |\dot{\gamma}_{\alpha}|.
\]

Here, \(h_{\alpha \beta}\) depends on the total slip rate \(\gamma\) as

\[
h_{\alpha \beta} = q_{\alpha \beta} h(\gamma),
\]
where
\[ q_{\alpha\beta} = \begin{pmatrix} A & qA & qA & qA \\ qA & A & qA & qA \\ qA & qA & A & qA \\ qA & qA & qA & A \end{pmatrix}, \quad A = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}. \quad (3.12) \]

Following (Nicola et al., 2008), a constant hardening rate \( h_0 \)
\[ h(\dot{\gamma}) = h_0. \quad (3.13) \]

is used.

The elastic part of the strain rate is specified by Hooke’s law,
\[ \dot{\varepsilon}_{ij} = \mathcal{L}_{ijkl} \dot{\varepsilon}_{kl}^e. \quad (3.14) \]

Here, \( \mathcal{L}_{ijkl} \) is the tensor of isotropic elastic moduli with Young’s modulus \( E \) and Poisson’s ratio \( \nu \).

For a fair comparison between the two models, the crystal plasticity parameters are chosen to fit the DD simulations for the uniaxial tension of a single crystal. DD simulations give an elastic perfectly plastic response, but in order to avoid numerical difficulties associated with non-hardening behavior in the continuum plasticity calculations, the hardening coefficient in most CP simulations is taken to be slightly larger than zero, \( h_0/E = 0.001 \). The initial critical strength \( \tau_0 \) for all slip systems is taken to be 50 MPa, i.e. equal to the average nucleation strength in the DD simulation. A reference slip rate of \( \dot{\gamma}_0 = 2 \times 10^3 s^{-1} \) is used and the rate sensitivity exponent in Eq. (3.9) is taken to be \( m = 0.005 \), which is a representative value for most FCC metals at room temperature, and which corresponds to practically rate independent behavior.

The same mesh is used for the CP and the DD simulations. In order to accurately capture the contact area and the dislocation fields, the mesh has very fine square elements with dimension of 3.2 nm at the surface of the crystal; the mesh gets coarser towards the bottom of the crystal.

### 3.3. Effect of asperity density

Simulations are performed for the flattening of surfaces with asperities of given size and shape, but at different spacing. Specifically, asperities of width \( w = 2 \mu m \) and amplitude \( A = 0.1 \mu m \) are considered, as well as self-similar larger asperities with \( w = 4 \mu m \) and \( A = 0.2 \mu m \). It has already been shown in (Sun et al., 2012) that asperities of this size exhibit a size dependent response, i.e. it is
3.3. Effect of asperity density

harder to flatten the large asperities than the small ones. For the small asperities, dislocation plasticity tends to be source limited, i.e. the availability of dislocation sources is not sufficient to sustain plastic deformation. Here, we will investigate the effect of the density of identical asperities and to this end consider spacings of \( s = 2, 4, 16 \) and \( 1000 \) \( \mu \)m.

3.3.1. Elasticity

Firstly, simulations are carried out for crystals without dislocation sources, in order to elucidate the effect of elastic interactions. In Fig. 3.2a the contact pressure \( P_m = F/C \), normalized by the plane-strain elastic modulus \( E^* = E/(1 - \nu^2) \approx 78.5 \) GPa is the biaxial elastic modulus, is plotted against asperity strain, defined as \( \varepsilon_a = (d_0 - d)/d_0 \) (see inset of Fig. 3.2). The choice of this strain definition, illustrated in Fig. 3.2b, is motivated by the fact that the effect of plasticity is most clearly visible when the solutions are elastically identical. When asperities are far apart, the elastic mean contact pressure as a function of asperity strain is indeed independent of spacing. However, when the asperity density is large, the mean contact pressure becomes dependent on spacing, as can be seen in Fig. 3.2a. When the spacing between asperities becomes comparable to their size, the elastic stress fields interact with each other (see Fig. 3.2b for the shear

\[
P_m = \frac{F}{C} = \frac{E^*}{1 - \nu^2} \approx 78.5 \text{ GPa}
\]

where \( E^* \) is the plane-strain elastic modulus and \( \nu \) is Poisson's ratio. The normalized contact pressure \( P_m \) is plotted against asperity strain \( \varepsilon_a \) for various spacing ratios \( s/w \) where \( s \) is the spacing between asperities and \( w \) is the wavelength of the asperities.

Figure 3.2: (a) The elastic contact pressure, normalized by the plane strain elastic modulus \( E^* \), as a function of asperity strain for asperities of wavelength \( w = 2 \) spaced at different distances. (b) Upper figure: sketch representing the asperity strain \( \varepsilon_a \); the dashed lines are the average height of the asperity before and after deformation, respectively. Note that \( d_0 = A \) for sinusoidal asperities. Middle and lower figures: the stress field \( \sigma_{12} \) at \( \varepsilon_a = 0.15 \) for \( w = 2 \) \( \mu \)m.
interaction between neighboring asperities during flattening stress at $\varepsilon_a = 0.15$).

It is important here to realize that, similarly to problems with high densities of microcracks or second-phase particles, an array of contacts is a problem where stress fields do not simply superpose and where strain gradients are significant. In fact, strain gradients very similar to those observed in indentation problems are to be expected, since the flattening of a sinusoidal surface gives rise to elastic fields as those of an array of equally spaced flat indenters at the same spacing.

### 3.3.2. Plasticity

The simulations presented above are now repeated after including the dislocation sources, and thus enabling the possibility of plasticity. Figure 3.3 shows the contact pressure during flattening for the smaller asperities $w = 2 \mu m$. When the spacing is $s = 16 \mu m$ or larger, the increase in contact pressure is essentially independent of asperity density. However, if the spacing between asperities is $s = 2 \mu m$, the response is harder. In fact, the asperity density effect that was observed above in elasticity appears to be magnified in the presence of plasticity. While for the elastic simulations in Fig. 3.2(a) the difference in contact pressure between close and spaced asperities, $\Delta P / E^*$, at a strain of $\varepsilon_a = 0.15$, is only 0.002, in the presence of plasticity the difference is 0.004 (these values correspond respectively to 4.4% and 17.4% of the pressure of the closer spaced asperities).

The fact that plasticity amplifies the asperity density effect can be attributed to one or a combination of the following effects: (a) plastic strain gradient effects of the type observed during nanoindentation (see, e.g., (Kreuzer and Pippan, 2007; Lou et al., 2003; Ma and Clarke, 1995; Nix and Gao, 1998; Pharr et al., 2010; Wijaja et al., 2007; Zong and Soboyejo, 2005)), (b) interaction between plastic zones, or (c) limited dislocation plasticity. Limited dislocation plasticity can have different origins: (1) dislocation starvation of the type observed in nanopillars (see, e.g., (Greer et al., 2005; Volkert and Lilleodden, 2006)), according to which too few dislocations are nucleated and (2) free path limited plasticity: there are many dislocations, but they interact with each other such that they cannot glide over sufficiently long distances to provide the required plastic deformation. In the remaining of this paper we will try to understand which of these effects are responsible for the asperity density effect.

Prior to this, however, we will verify that the asperity density effect vanishes when all the aforementioned possible causes are absent. This is the case of CP simulations: since they are based on a local plasticity theory, these simulations cannot capture any strain gradient effect. Also, since continuum theory presumes that plasticity is available whenever and wherever it is needed, dislocation limi-
3.3. Effect of asperity density

Figure 3.3: The normalized contact pressure as a function of asperity strain for various spacings between asperities of wavelength $w = 2$. Each curve is the average over six realizations of the positions of the obstacles and dislocation sources.

The interactions between plastic zones cannot be excluded a-priori, but this is what we find in CP simulations with no hardening, as shown in Fig. 3.4(b). As expected, these simulations are insensitive to asperity spacing and give the same response for all asperity densities considered. Since there is no material hardening, the average pressure predicted by these CP simulations is significantly lower than that predicted by any of the DD simulations. It is noted that the onset of plasticity occurs much earlier than in the DD simulations, and thus at a strain where the elastic interaction is still negligible. The reason for the difference in the onset of plasticity between DD and CP is that in the DD simulations plasticity occurs only when a source experiences a sufficiently large Peach–Koehler force to nucleate. Even if there is a very high stress state below the contact region, nucleation does not take place if none of the dislocation sources are sufficiently close to that region. On the contrary, plasticity occurs in CP whenever the slip system strength is exceeded.

For the simulations in Fig. 3.3 the distribution of stress $\sigma_{22}$ and dislocations in widely versus closely spaced asperities at the asperity strain $\varepsilon_a = 0.25$ are presented in Fig. 3.4. A few observations can be made: in the DD results the density of dislocations is rather large, indicating that dislocation starvation is unlikely to play a major role in the asperity density effect. Dislocations are mainly located just underneath the contact. This means that for the widely separated asperities there are wide regions in between asperities that are dislocation free (see Fig. 3.4(a)). On the contrary, when the asperities are proximate (see Fig. 3.4(b)) the disloca-
Figure 3.4: The middle figures show the stress $\sigma_{22}$ and dislocation distribution at the asperity strain of 0.25 for asperities (a) widely separated (at $s = 16$ $\mu$m) and (b) closely spaced (at $s = 2$ $\mu$m). The bottom figures show the corresponding stress states obtained by crystal plasticity simulations. The top figures represent the contact pressure profiles obtained by DD (in red) and by CP (in blue). The stress is normalized by the yield strength $\sigma_Y \approx 50$MPa of the single crystal. The dashed lines represent the average contact pressure in the DD simulations.

Dislocations are rather homogeneously distributed at the top of the crystal. It is no longer possible to distinguish from which contact the dislocations have been generated. This suggests that interaction between neighboring plastic zones or limitation of the mean–free path of dislocations might be significant.

The stress state predicted by DD in the case of closely spaced contacts is remarkably different from that obtained by CP simulations (as shown at the bottom of Fig. 3.4): a highly compressive stress state is present in the upper two microns of the crystal according to DD, while according to CP only the region just below each asperity is highly stressed. This observation again indicates that interaction between neighboring plastic zones is probably relevant in DD. The stress state predicted by CP and DD for the crystals with widely spaced asperities is more similar in an average sense, but the local pressure at the contact, shown in the upper part of the figure is very different. The pressure profile is almost uniform according to the CP predictions but highly inhomogeneous according to DD, in agreement with our previous findings for sinusoidal surfaces (see (Sun et al., 2012)). Notice also that the stress peaks are remarkably high, up to 200 times the yield strength.
These results indicate, in agreement with (Gao and Bower, 2006), that the asperities are persistent and can support very high loads without flattening.

Effect of source spacing

To gain a better understanding of the role of plasticity in the asperity density effect we here analyse the effect of source spacing on contact pressure. Simulations are performed for asperities with size $w = 2 \, \mu m$ and $A = 0.1 \, \mu m$, with a constant obstacle spacing, $L_{obs} = 0.18 \, \mu m$, but different source spacings: $L_{nuc} = 0.09$, 0.13, 0.26 and 1 $\mu m$.

![Graph showing normalized contact pressure as a function of asperity strain for different source spacings.](image)

The differences in contact pressure, see Fig. 3.5(a), between differently spaced asperities $\Delta P_m / E^*$ is 0.004, 0.004, 0.002, 0.001 for a source spacing of 1, 0.26, 0.13 and 0.09 $\mu m$, respectively. We know from Fig. 3.2 that this difference is 0.002 in the elastic limit. This limit is approached for source spacings wider than 1 $\mu m$ and not reported here; a maximum in the spacing effect is expected for a source spacing between $L_{nuc} = 1$ and 0.26 $\mu m$; and for decreasing source spacing the asperity density effects decreases until convergence to the continuum plasticity limit.

These observations may trigger the question: what is the continuum plastic limit? Does it represent no asperity density effect at all, similarly to the CP simulations in Fig. 3.3? The answer to this question is no: the asperity density effect depends on hardening, also in the limit of continuum plasticity. This can be seen in Fig. 3.5(b), where the effect of the hardening coefficient in CP simulations is
presented for the two asperity densities. For $h_0/E = 0.01$ the curves for close and widely spaced asperities almost overlap. Thus, only if the hardening coefficient approaches zero the asperity density effect vanishes. For increasing hardening the asperity density effect found in elasticity is approached (but never exceeded). The origin for an asperity density effect in CP can only be interaction between plastic zones (there are no plastic strain gradients, nor limits on dislocation plasticity). Indeed, as can be seen in Fig. 3.6, plastic zones represented by regions where the resolved shear stress in the $\varphi = 60^\circ$ direction (the direction of the slip plane in the DD simulations) exceeds 50 MPa do overlap when the hardening coefficient is large.

Thus, we conclude that when plastic deformation is carried by discrete dislocations with a source spacing of about $L_{nuc} = 0.26 \mu m$ the asperity density effect is enhanced with respect to both the elastic and the continuum plastic limits. Why is this the case? Limited dislocation plasticity must be somehow involved. To better understand in which way, in the next section we will study the case of large asperities, where dislocation plasticity is expected to be less restricted.

3.3.3. Effect of asperity size

In order to investigate how the asperity density effect is affected by asperity size, simulation results are reported here for asperities with $w = 4 \mu m$, spaced at $s = 4 \mu m$ and $s = 16 \mu m$. The contact pressure during loading is shown in Fig. 3.7(a) together with the results obtained in the previous section for the smaller asperities. As expected, the response is size dependent: the large asperities are easier to flatten than the small asperities (cf. (Sun et al., 2012)). For large asperi-
ties it is found that there is no asperity density effect, independently of dislocation source spacing (see Fig. 3.7(b)). This is consistent with the fact that plasticity in large asperities is less likely to be source limited than in small asperities, and therefore dislocation limitation is not an issue. Moreover, the actual spacing between contacts is twice as large as in small asperities, thus interaction of plastic zones is not expected.

Figure 3.8 shows that also for the large asperities the contact area is discontinuous and the pressure profiles have similar localized high peaks. In fact, the contact areas for the larger asperities are even more discontinuous than those for the smaller asperities, for all spacings. This is because the surfaces have a different geometry: the asperity profile is less steep, which implies that it is easier for a larger asperity to create new contact segments caused by material pile-up due to dislocations gliding out of the free surface. However, the exact shape of the contact, more or less patchy, does not affect the asperity density effect. In fact, the shape and size of the stress field underneath a continuous contact or a patchy contact are almost indistinguishable when loaded to the same displacement, as can be seen in Fig. 3.9. The figure highlights in red and blue the regions where the stress resolved on the $\varphi = 60^\circ$ direction (the direction of the slip plane in the DD simulations) is larger than the average nucleation strength of the dislocation sources, $\tau_{nuc} = 50$ MPa. Differences are visible only very close to the surface in a region that is anyhow too small to contain a significant number of sources or to
3. Interaction between neighboring asperities during flattening

Figure 3.8: The upper figures are the contact pressure profiles for different surfaces at the asperity strain of 0.25 for (a) $w = 4 \, \mu m$, $s = 16 \, \mu m$, (b) $w = 4 \, \mu m$, $s = 4 \, \mu m$, with dashed lines being the average contact pressure, while the middle figures are the corresponding stress distribution $\sigma_{22}$ and the bottom figures are the corresponding results for the CP simulations.

sensibly affect strain gradients or plastic interaction.

Figure 3.9: The elastic shear stress resolved along the 60° direction for (a) a continuous contact area and (b) a patchy contact area.
3.4. Discussion and conclusions

Two-dimensional discrete dislocation plasticity simulations are performed for the flattening of a single crystal with rough surface, represented by equally spaced sinusoidal asperities. The goal of this work is to investigate the dependence of plastic flattening on the spacing between neighboring asperities.

Firstly, it was noticed that an asperity density effect, with widely separated asperities being easier to be flattened than closely spaced ones, is already present in purely elastic materials because the fields do not superpose.

Secondly, the asperity density effect becomes larger when plasticity is described by discrete dislocations. This effect strongly depends on the average spacing between dislocation sources $L_{\text{nucl}}$. For very small source spacings (i.e. a very high source density), the asperity density effect is very small to vanishing, similarly to what is found when using continuum crystal plasticity. For increasing source spacings (i.e., decreasing source density), the asperity density effect increases up to a maximum, after which it decreases until the elastic limit is approached.

The origin of the asperity density effect is a combination of plastic strain gradients, dislocation limited plasticity and interaction between plastic zones. Plastic strain gradients are inevitably present, since the flattening problem is similar to that of an array of indenters. However, the effect of plastic strain gradients is tightly bound to the available amount of dislocation glide. Only when the source spacing is large, strain gradient effects become apparent. If there are sufficiently many sources for dislocations, dislocation glide diminishes the effect of strain gradients. Limited dislocation plasticity is a cause for additional hardening and amplifies the effect of strain gradients. Here, by limited dislocation plasticity we refer to the fact that dislocations, despite being present in a large number, cannot provide as much glide as required, everywhere where required by the gradients. This is different from dislocation starvation of the type found in nanopillars, since in our simulations dislocation densities are rather high, for any asperity density. In fact the dislocation density is so high that the dislocations form many entanglements with other dislocations, thus reducing their free path. Limited dislocation plasticity goes hand in hand with strain gradient effects. This is true even for individual contacts (Widjaja et al., 2007). For arrays of contacts, interaction between plastic zones is an additional effect, which strengthens the other two.

Additionally it is observed, in agreement with (Gao and Bower, 2006; Sun et al., 2012), that the asperities in these simulations are highly persistent, they reach local pressure up to a couple of order of magnitude larger than the material hardness.
References


Effect of flattening on the shearing response of metal asperities

Discrete dislocation 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.

4.1. Introduction

In all problems of interest to tribology, surfaces need to firstly 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 (Majumdar and Bhushan, 1990), and by the material properties.

Experimental flattening of a spherical asperity (Jamari and Schipper, 2006) as well as multiasperities (Jamari et al., 2007) show 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 (Müser, 2008; Persson, 2001). 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 (Majumdar and Bhushan, 1991). 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 microindentation of metal surfaces (Lou et al., 2003; Nix and Gao, 1998; Pharr et al., 2010; Zong and Soboyejo, 2005), 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 discrete dislocation plasticity, which can capture possible size and strain gradient effects, if present. This is possible because in the discrete dislocation plasticity description dislocations are individually modeled. Besides the Burgers vector of the dislocations, this introduces other materials length scales, which can make its predictions size dependent. Indeed, an analysis of the flattening of surfaces with sinusoidal asperities (Sun et al., 2012, 2015) showed that the contact pressure increases with reduced asperity size and increases when the density of contacts is increased.

In this study we take the next step and aim to understand to which extent plastic deformation of asperities during normal loading affects their subsequent plastic shearing. Will dislocations generated during contact facilitate or hinder subsequent plastic shearing? Also we investigate the effect of asperity spacing on the shearing behavior of the asperities. Since it was found that a large asperity density requires a larger pressure to be flattened, the question arises on whether it is easier or more difficult to shear closely spaced contacts than widely separated.
The relation between the contact area of elastically deforming single asperities and load is found to be non-linear (Archard, 1957); however, this relation appears to be linear when multiple asperities of different geometries are considered (Bowden and Tabor, 1950, 1964). In this study, to simplify the problem, only asperities with rectangular shape are analyzed. In this way, the contact area is constant during both flattening and shearing. The effect of normal loading on the subsequent shearing is then explored.

4.2. Formulation

4.2.1. Boundary value problem

We perform two-dimensional simulations of flattening and shearing for a single asperity protruding from a single crystal, illustrated in Fig. 5.1. The crystal has a length of \( L = 1000 \ \mu\text{m} \) and height \( h = 50 \ \mu\text{m} \). The asperity has a rectangular shape with width \( w \) and height \( h_p \). Dislocations can nucleate and glide in the asperity and in a region below the asperity of dimensions \( L_{pl} = 60 \ \mu\text{m} \) and \( H_{pl} = 15 \ \mu\text{m} \). The loading consists of two steps: first the asperity is flattened by prescribing vertical displacement of the contact to a certain displacement, then the asperity is sheared. Flattening is imposed by prescribing

\[
u_2(x_1, h + h_p) = \int v_2 \, dt, \quad x_1 \in \left[ \frac{L - w}{2}, \frac{L + w}{2} \right],
\]

where \( v_2 \) 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

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Figure 4.1: Two-dimensional model of an asperity on a larger crystal flattened and sheared by a rigid platen (the dimensions are not to scale). The rigid platen is drawn only as illustration and its influence on the asperity is simply accounted for by means of boundary conditions.
frictionless:
\[ \sigma_{12}(x_1, h + h_p) = 0, \quad x_1 \in \left[ \frac{L - w}{2}, \frac{L + w}{2} \right], \quad (4.2) \]
or sticking:
\[ u_1(x_1, h + h_p) = 0, \quad x_1 \in \left[ \frac{L - w}{2}, \frac{L + w}{2} \right]. \quad (4.3) \]
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
\[ u_1 = u_2 = 0, \quad \text{for} \quad x_1 = 0 \quad \text{or} \quad x_1 = L. \quad (4.4) \]
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
\[ u_1(x_1, h + h_p) = \int v_1 \, dt, \quad x_1 \in \left[ \frac{L - w}{2}, \frac{L + w}{2} \right], \quad (4.5) \]
\[ u_2(x_1, h + h_p) = u_0, \quad x_1 \in \left[ \frac{L - w}{2}, \frac{L + w}{2} \right], \quad (4.6) \]
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,
\[ u_1 = u_2 = 0, \quad \text{on} \quad x_2 = 0. \quad (4.7) \]

4.2.2. Discrete dislocation plasticity

The discrete dislocation (DD) plasticity method by Van der Giessen and Needleman (Van der Giessen and Needleman, 1995) 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
4.3. The effect of normal loading on plastic shearing

4.3.1. Large asperities

To investigate the effect of the applied contact pressure on the subsequent shearing, asperities with size \( w = 4 \mu m \) and \( h_p = 2 \mu m \) are firstly compressed to three values of the flattening depth, i.e. \( u_z = 0.0012, 0.012 \) and \( 0.02 \mu m \), and

spacing \( L_{nuc} \) and \( L_{obs} \), respectively. Dislocation dipoles are generated when the shear stress on a source is larger than the nucleation strength, \( \tau_{nuc} \). There are two other parameters that are related to nucleation: the time, \( t_{nuc} \), required for formation of the dipole and the spacing between the newly generated dislocations, \( L_{dis} = Gb/2\pi(1 - \nu)\tau_{nuc} \), where \( G \) is the shear modulus, \( b \) is the Burgers vector and \( \nu \) is the Poisson's ratio. The glide velocity \( v^l \) of the \( j \)th dislocation is proportional to the Peach-Koehler force \( f^l \), according to \( v^l = f^l/B \) 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, \( \tau_{obs} \).

4.2.3. Material parameters

The crystal is taken to have the elastic properties of aluminum with Young's modulus \( E = 70 \) GPa and Poisson's ratio \( \nu = 0.33 \). Following Rice (Rice, 1987), the FCC crystal is modeled in two dimensions by considering three potentially active slip systems. In these simulations the slip planes are oriented at \( \varphi = 15^\circ, 75^\circ \) and \( 135^\circ \). 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 \( 60^\circ \) with each other. This is a few degrees different from the real orientation of planes in an FCC crystals, as described in (Rice, 1987), but this difference will not noticeably affect our results. The spacing between slip planes in the crystal is \( 200b \), where the magnitude of the Burgers vector being \( b = 0.25 \) nm. The average critical strength of the sources is taken to be \( \bar{\tau}_{nuc} = 50 \) MPa, with a 20% standard deviation. The average source spacing \( L_{nuc} \) is \( 0.13 \mu m \), while the average obstacle spacing \( L_{nuc} \) is \( 0.18 \mu m \), unless stated otherwise. The time span necessary for nucleation of a dislocation dipole, \( t_{nuc} \), is 10 ns.

The mesh is made of very fine \( 5 \) \( nm \times 5 \) \( nm \) 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 \( 0.02 \mu m \) underneath the contact to prevent exit of dislocations from the contact.
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 4.2](image)

Figure 4.2: (a) The mean contact pressure and total dislocation density during flattening under different contact conditions for the asperity with \( w = 4 \, \mu \text{m} \) and \( h = 2 \, \mu \text{m} \). The letters A, B and C represent the points on the loading curve when the shearing starts. (b) The contact shear stress as a function of tangential displacement during shearing.

Figure 5.2a 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 \( u_2 = 0.006 \, \mu \text{m} \), 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. 5.2a by the letters A, B and C, the asperity is sheared up to \( u_1 = 0.03 \, \mu \text{m} \) with perfect sticking contact conditions. Figure 5.2b 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 plasticly 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 dif-
Figure 4.3: The stress state $\sigma_{12}$ and dislocation distribution for frictionless contact at flattening depths (a) $u_2 = 0.0012 \, \mu m$ (corresponding to point A in Fig. 5.2a) and (b) $u_2 = 0.02 \, \mu m$ (corresponding to point C), after shearing to $u_1 = 0.01 \, \mu m$ starting from a flattening depth (c) $u_2 = 0.0012 \, \mu m$ (corresponding to point A) and (d) $u_2 = 0.02 \, \mu m$, and after shearing to $u_1 = 0.03 \, \mu m$ starting from a flattening depth (e) $u_2 = 0.0012 \, \mu m$ and (f) $u_2 = 0.02 \, \mu m$.

Different plastic shearing mechanism than that occurring when shearing a dislocation free crystal. Figure 4.3a and b show on the left hand side 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. 5.2a) and on the right hand side the crystal flattened to $u_2 = 0.02 \, \mu m$ (corresponding to point C in Fig. 5.2a). 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. Figure 4.3c and d show the stress state $\sigma_{12}$ after shearing by $u_1 = 0.01 \, \mu m$. For this tangential displacement the difference
in shear stress is the largest according to Fig. 5.2b. By contrasting Fig. 4.3c with d it is possible to observe two different mechanisms: plasticity in the crystal which started from the dislocation-free state (left figure) is confined to the asperity, while the crystal on the right presents a deep shear band that indicates shearing of the subasperity region. The bottom figures represent shearing at \( u_1 = 0.03 \mu m \), when the shear stress-displacement response of both crystals is similar. In both cases subasperity plasticity has taken place.

Figure 4.4 shows the \( \sigma_{12} \) stress profiles at contact after only flattening (4.4a) and after flattening and shearing (4.4b). The shear stress on the contact surface is zero everywhere for the frictionless contact at the final flattening depth, while for the sticking contact, there is a high contact shear stress on both sides of the contact, i.e. both locations are equally likely to initiate sliding 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. 4.4b. 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 \( u_2 = 0.012 \mu m \) (B) or \( 0.02 \mu m \) (C) and then unloaded to points M and N, respectively, see Fig. 4.5a. The residual amounts of deformation are about 0.0015 \( (\mu m) \) and 0.008 \( (\mu m) \), respectively. The shear-
The effect of normal loading on plastic shearing

Figure 4.5: (a) The mean contact pressure during flattening and unloading under sticking contact conditions for the asperity with $w = 4 \, \mu m$ and $h_p = 2 \, \mu m$. 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.

Figure 4.6: The stress state $\sigma_{zz}$ and dislocation distribution for sticking contact when the asperity is totally unloaded from flattening depths (a) $u_2 = 0.012 \, \mu m$ and (b) $u_2 = 0.02 \, \mu m$.

4.3.2. Small asperities

Simulations were also performed for a rectangular asperity, $w = 0.8 \, \mu m$, $h_p = 0.4 \, \mu m$ 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 the previous section.

Notice that care must be taken in comparing the results with those for the large asperity above, since the elastic response is different.

![Figure 4.7](image)

Figure 4.7: (a) The normal mean contact pressure and total dislocation density during flattening under sticking contact conditions for a pillar with \( w = 0.8 \mu m, h_p = 0.4 \mu m \). 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.

Figure 4.7a 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. 5.2a. 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 of single crystals (Balint et al., 2006). The main reason for the difference is that the loading affects 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 (Dikken et al., 2015). Figure 4.7b 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. 4.7a. 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 realisations.

Figure 4.8 shows the stress state \( \sigma_{12} \) and the dislocation distribution at various
The effect of normal loading on plastic shearing

Figure 4.8: The stress state $\sigma_{12}$ and dislocation distribution for the asperity with $w = 0.8 \, \mu m$, $h_p = 0.4 \, \mu m$, 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 $u_2 = 0.02 \, \mu m$.

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 nucleated during flattening (see Fig. 4.8b) they do not contribute to facilitate shearing, as evident from Fig. 4.7. Figures 4.8c and 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. 4.7). This is a clear indication that the dislocation density, which is often calculated numerically or experimentally as a measure of plastic activity, bares little relation with it. Compared to the case of large asperity, the dislocation density in the asperity of Fig. 4.8d 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.
4.3.3. 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 the previous section. Figure 4.9a shows the mean contact pressure as a function of flattening depth. As to be expected, elastic asperities require a larger contact pressure to be flattened. Figure 4.9b 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.

4.4. Effect of asperity spacing

In this section we investigate the effect of the spacing between asperities on the shearing response. In our previous study (Sun et al., 2015), 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...
4.4. Effect of asperity spacing

crystal of the type analyzed in the previous sections, but with three asperities protruding from its surface spaced at \( s_p \), as illustrated in Fig. 4.10. Simulations of flattening and shearing are performed on asperities with dimensions \( w = 0.8 \) \( \mu m \), \( h_p = 0.08 \) \( \mu m \) spaced at \( s_p = 0.4 \) \( \mu m \), \( s_p = 2.0 \) \( \mu m \), and \( s_p = 8.0 \) \( \mu m \). The crystal has the same length of \( L = 1000 \) \( \mu m \) and height \( h = 50 \) \( \mu m \) as in previous sections. 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 4.10: Two-dimensional model of three asperities on a larger crystal flattened and sheared by a rigid platen.](image)

Figure 4.10 shows the contactshear traction of the middle asperity as a function ofasperity shear strain. As illustrated in the inset of in Fig. 4.11a the asperity shear strain is defined as \( \gamma = u'/h' \), where \( h' \) is the height of the flattened asperity and \( u' = u_1 - u_b \). Here, \( u_1 \) is the tangential displacement at the top of the asperity.

![Figure 4.11: (a) The elastic shear response of the middle pillar and a sketch that illustrates the definition of strain. (b) The shear traction of the middle pillar as a function of shear strain for different spacings.](image)
and $u_b$ 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. 4.11b 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 (Sun et al., 2015): increasing the asperity density hinders plastic flattening, while it is here found that it facilitates plastic shearing. The light blue curve in Fig. 4.11b indicates the results for a single asperity whose width is equal to the size of the asperities, i.e. $w = 2.4 \ \mu m$.

Figure 4.12a and b show the stress state $\sigma_{12}$ 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.

![Figure 4.12: Stress state $\sigma_{12}$ and dislocation structure of three asperities with $w = 0.8 \ \mu m$ at shear strain $\gamma = 0.008$ for different spacings. (a) $s_p = 8.0 \ \mu m$ and (b) $s_p = 0.4 \ \mu m$.](image)

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 on it, as can be seen in Fig. 4.13. 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 (Sun et al., 2015) it is to be expected
4.4. Effect of asperity spacing

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 $h_p/w = 0.5$ yet the same width $w = 0.8 \ \mu m$. Figure 4.14 shows the shear traction as a function of shear strain for asperities with different spacing. The shear tractions are almost the same, indicating that there is no plastic interaction between tall asperities.

This is confirmed in Fig. 4.15a and 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.

4.4.1. Effect of normal loading on multiasperity shearing

The preloading in the normal direction has been found in Sec. 4.3 to affect the shearing behavior of large pillars. In this section, the effect of preloading on multiasperities 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 4.16a for the shear stress as a function of shear strain shows that the asperity spacing effect is reduced by plastic flattening. This is
4. Effect of flattening on the shearing response of metal asperities

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 4.16b shows the shear stress as a function of shear strain for this protruding asperity. The spacing effect is absent and therefore independent of preloading.
4.5. Conclusions

Discrete dislocation 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.

- 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.

- 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.

References


Discrete dislocation plasticity simulations are performed to investigate the static frictional behavior of a metal asperity on a large single crystal, in contact with a rigid platen. The focus of this study is on understanding the relative importance of contact slip opposed to plasticity in a single asperity at the micrometer size scale, where plasticity is size dependent.

Slip of a contact point is taken to occur when the shear traction exceeds the normal traction at that point times a microscopic friction coefficient. Plasticity initiates through the nucleation of dislocations from Frank-Read sources in the metal and is modeled as the collective motion of edge dislocations.

Results show that plasticity can delay or even suppress full slip of the contact. This generally happens when the friction coefficient is large. However, if the flattening depth is sufficiently large to induce nucleation of a large dislocation density, slip is suppressed even when the friction coefficient is very small. This study also shows that when self-similar asperities of different size are flattened to the same depth and subsequently loaded tangentially, their frictional behavior appears size independent. However, when they are submitted to the same contact pressure, smaller asperities slip while larger asperities deform plastically.

The Chapter is submitted to Acta Mater., as “Dry frictional contact of metal asperities: a dislocation dynamics analysis” by Sun, F., Van der Giessen, E., Nicola, L.
5.1. Introduction

Friction between two rough surfaces resists their relative motion. The surfaces respond to an applied sliding force by deforming elastically and plastically and by eventually loosing adhesion. Plastic deformation and loss of adhesion are competing mechanisms: if the contact roughness can respond to the applied load through plastic deformation, slip at the interface might not take place, albeit at the macroscale the bodies appear displaced relative to each other. The occurrence of slip will clearly depend also on the interfacial energy between the contacting surfaces, and therefore on the materials in contact.

The classical Amontons–Coulomb law of friction states that sliding of a macro-scale contact occurs when the ratio between the tangential force $f$ and the applied normal force $f_n$ exceeds the friction coefficient $\mu$. This statement relies on the assumption that the friction coefficient $\mu$ is a constant and therefore a property of the interface, and that it is not important how the friction force and the normal force vary along the contact, since only forces averaged along the contact are considered. Along the same line, Bowden and Tabor (Bowden, 2001) stated that the friction force is proportional to the true contact area $C$, where the proportionality constant is the friction strength. Again, variations in the shear stress along the contact are not assumed to be significant or relevant in the friction process.

However, when two surfaces are under contact loading, it has been shown by molecular dynamics (Luan and Robbins, 2005) and discrete dislocation plasticity simulations (Deshpande et al., 2004) that the contact shear stress varies significantly along the apparent contact area. This is mainly attributed to the fact that the true contact area is highly patchy at the micrometer scale. Experimentally, contact stress profiles cannot yet be measured, even though Bonn and coworkers (Suhina et al., 2015) have recently devised a very interesting experimental technique that holds the promise of making it possible in the near future. The method is based on the enhancement of the fluorescence of rigidochromic probe molecules attached to one of the contacting surfaces. Results obtained by this method for a plastic sphere in contact with a flat glass surface confirm that the contact area is patchy. Consequently, it is to be expected that the contact pressure profile is indeed a collection of high peaks, instead of a smooth pressure distribution as is predicted by continuum plasticity simulations, e.g. (Gao et al., 2006).

The aim of this paper is to investigate the frictional behavior of a single microscale asperity protruding from the surface of a metal body, accounting for plasticity. Plastic deformation has been observed experimentally when flattening spherical single (Jamari and Schipper, 2006) and multi-asperities (Jamari et al., 2007).
with moderate contact loads. The numerical technique used in this study is the discrete dislocation plasticity method (Van der Giessen and Needleman, 1995) which can capture key features of microscale plasticity: size effects (Nicola et al., 2003, 2005; Polonsky and Keer, 1996), strain gradient effects (Cleveringa et al., 1999; Kreuzer and Pippan, 2007; Widjaja et al., 2007) as well as local stress peaks in the surface pressure (Polonsky and Keer, 1996; Sun et al., 2012). Attention here will mainly focus on the competition between plasticity and slip, for micron-scale asperities of different size.

This work is an extension of previous discrete dislocation plasticity studies where a single or multiple asperities were plastically sheared, under sticking contact conditions (Dikken et al., 2015; Sun et al., 2015). Due to the full sticking nature of the contact, a very high shear stress was reached locally on the contact. Here, we use a contact condition that, instead, allows for local sliding. Inspired by the Cattaneo-Mindlin problem (Cattaneo, 1938; Mindlin, 1949), the contact will slip when the contact shear stress exceeds the normal shear stress multiplied by a constant friction coefficient. The difference with the Cattaneo-Mindlin problem and with the classical Amonton’s law is that instead of using average stresses on the contact, local stresses will be computed at each point in contact. For simplicity in the interpretation of the results, the asperities are firstly flattened with a rigid platen, such as to reach elastic or plastic deformation, and subsequently loaded tangentially by rigidly displacing the platen. Also, the asperity is taken to be flat initially, so that the contact area stays constant during the simulation. This choice is motivated by the fact that flattening asperities with sinusoidal profile leads to a highly fragmented contact area, with a large central contact region surrounded by many small contact patches. The contact patches are a consequence of dislocations leaving behind crystallographic steps at the surface (Sun et al., 2012). Using such a fragmented contact area as the starting point for the shearing simulations has the drawback that the size of the small contact patches can be an order of magnitude smaller than the large contact area, and therefore the question arises on whether the various contact patches should have the same friction coefficient, and if not, how much should they differ. Additionally, the size and location of the contact patches is stochastic and obtain statistically significant results would require a large number of simulations.

A similar modeling approach for dry static friction was used by Deshpande et al. (Deshpande et al., 2007) who investigated the behavior of flat and sinusoidal microscale contacts on a flat metal single crystal. The contact was mimicked by means of a cohesive zone. De-adhesion of the interface was modeled via a shear traction versus tangential displacement relationship, which is characterized by a
cohesive strength, independent of the normal load acting on the contact. The paper (Deshpande et al., 2007) has the merit of showing that the friction stress is dominated by slip at small contact size (smaller than $\approx 40 \text{ nm}$), and by plasticity at large contact size (larger than $\approx 4 \mu\text{m}$). However, the assumption that the cohesive strength $\tau$ is independent of both contact size and normal loading, leads to very high friction coefficients ($\mu = \tau/P$ reaches values much above 10 in (Deshpande et al., 2007)). It should be noted that this is not in conflict with the Bowden-Tabor interpretation of the friction force being the product of friction strength and contact area, because they assumed that the contact area increases with increasing normal loading. Nevertheless, in order to avoid any possible confusion on this, we here introduce a friction coefficient that relates the shear traction to the local contact pressure.

5.2. Formulation
5.2.1. Boundary value problem

A rigid platen is in contact with a large metal single crystal through a single rectangular asperity that protrudes from the surface of the metal crystal (see Fig. 5.1). The length of the crystal is $L = 1000 \mu\text{m}$ and its height $h = 50 \mu\text{m}$. The loading consists of two steps: first the asperity is flattened by prescribing vertical displacement of the rigid platen, then the platen is displaced tangentially. During flattening,

$$u_2(x_1, h + h_p) = -\int_C v_2 \, dt,$$

where $v_2$ is the velocity of the rigid platen in the vertical direction and $C := [-w/2, w/2]$ is the contact area. Outside the contact region, the top surface is traction free. The
boundary conditions at the bottom are:

\[ u_1 = u_2 = 0, \quad \text{on} \quad x_2 = 0. \] (5.2)

The traction distribution along the contact normal to the platen determines the flattening force \( F_n \) (per unit of out-of-plane depth):

\[ F_n := - \int_{C} \sigma_{22} dx_1. \] (5.3)

Similarly, the shear force is calculated as

\[ F_s := \int_{C} \sigma_{12} dx_1. \] (5.4)

After flattening, a tangential displacement is imposed at the contact by prescribing

\[ u_1(x, h + h_p) = \int_{C} v_1 dt, \]

\[ u_2(x, h + h_p) = u_0, \quad x_1 \in C, \] (5.5)

(5.6)

where \( v_1 \) is the velocity of the platen in the horizontal direction and \( u_0 \) is the flattening depth obtained after normal loading. However, if at any contact point

\[ |\frac{\sigma_{12}}{\sigma_{22}}| \geq \mu, \] (5.7)

where \( \mu \) is the local friction coefficient, de-adhesion is assumed to occur and the boundary condition in Eq. (5.5) is replaced with

\[ f(x, h + h_p) = \text{sign}(\sigma_{12})\mu|f_n(x_1, h + h_p)|. \] (5.8)

For the contact to slip fully the condition in Eq. (5.7) needs to be satisfied everywhere along the contact.

During tangential loading, part of the surface may be subjected to tension. Since the contact can slip, it is realistic to expect that the contact can detach in the normal direction when a critical separation strength \( \sigma_s \) is reached. However, since we cannot estimate this critical value we will assume that the contact detaches in the normal direction as soon as it is under tension.
5.2.2. Discrete dislocation plasticity

The simulations are performed using the discrete dislocation (DD) plasticity method proposed by Van der Giessen and Needleman (Van der Giessen and Needleman, 1995). The stress, strain, and displacement fields of the dislocated crystal are calculated making use of the superposition of elastic fields. The analytical elastic solution for the dislocations in an infinite medium is superposed to the numerical correction for the image field that takes the boundary conditions into account. The image fields are here solved by finite elements. The finite element mesh is made of very fine square elements with dimensions of 1.25 nm at the surface of the crystal to capture the contact stress distribution, while the mesh is coarser at the bottom of the crystal. The crystal is taken to have the elastic properties of aluminum with Young’s modulus $E = 70$ GPa, shear modulus $G = 26$ GPa and Poisson’s ratio $\nu = 0.33$.

Inspired by Rice (Rice, 1987), the FCC crystal is modeled in two dimensions by considering three potentially active slip systems that are oriented at $60^\circ$ relative to each other; the crystal is oriented such that the slip planes are at $\varphi = 15^\circ$, $75^\circ$ and $135^\circ$ relative to the crystal surface. The spacing between slip planes in the crystal is $200b$, where $b$ is the magnitude of the Burgers vector ($b = 0.25$ nm).

The development of the dislocation structure on the slip planes in the crystal follows constitutive rules that incorporate nucleation, glide and annihilation of dislocations, as well as pinning at obstacles. The simulation starts from a dislocation free state. The crystal contains a given density of dislocation sources and obstacles. Dislocation dipoles form when the shear stress on a source is larger than its strength. The average strength of sources is taken to be $\bar{\tau}_{nuc} = 50$ MPa, with a 20% standard deviation. Two other parameters which are related to nucleation are the time $t_{nuc}$ required for its formation and the spacing between dislocations at nucleation, $L_{dis} = Gb/2\pi(1 - \nu)\tau_{nuc}$. The glide velocity $v^l$ of the $I$th dislocation is proportional to the Peach–Koehler force $f^l$, according to $v^l = f^l / B$ where $B$ is the drag coefficient. Point obstacles are included in the simulation to represent small precipitates in the material where dislocations can be pinned, as long as the Peach–Koehler force on the pinned dislocation at the obstacles is less than $b$ times their strength, $\tau_{obs} = 150$ MPa. Impenetrable obstacles which are put 20 nm underneath the contact prevent dislocations to exit the contact. The average source spacing $L_{nuc}$ is taken to be 0.13 $\mu$m, while the average obstacle spacing $L_{obs}$ is 0.18 $\mu$m, unless stated otherwise. The time span necessary for nucleation of a dislocation dipole, $t_{nuc}$, is 10 ns.
5.3. Flattening of the asperity

A n asperity with dimensions \( w = 4 \mu m \) and \( h_p = 2 \mu m \) is flattened to \( u_2 = 0.012 \mu m \). The friction coefficients chosen for these simulations are \( \mu = 0.1, 0.3 \) and \( 0.7 \), which cover a range of experimental friction coefficients for engineering materials\(^1\). The upper limit of the realm of friction coefficients, i.e. a full sticking contact, is studied in (Dikken et al., 2015) and the lower limit, frictionless, is evidently meaningless. The simulations are first performed under fully elastic conditions, i.e. without dislocation sources, to be able to better assess the effect of plasticity through comparison.

5.3.1. Elastic results

![Stress profiles](a) \( \sigma_{22} \), (b) \( \sigma_{12} \) and (c) the horizontal displacement of the contact of an asperity with \( w = 4 \mu m \) and \( h_p = 2 \mu m \) at the final flattening depth \( u_2 = 0.012 \mu m \) for different friction coefficients.

Results in terms of normal and shear stress at the contact and the horizontal displacement of the contact, at final displacement, \( u_2 = 0.012 \mu m \), are presented in Fig. 5.2. The stress profile \( \sigma_{22} \) in Fig. 5.2a is hardly sensitive to the friction coefficient, contrary to the contact shear stress \( \sigma_{12} \) (see Fig. 5.2b) which is approximately constant in the slipped region when \( \mu = 0.1 \). It should be noted that the stress \( \sigma_{12} \) upon slipping is \( \mu \sigma_{22} \), where \( \mu \) is constant. Since the stress \( \sigma_{22} \) is very high at the corners of both sides of the contact, also the contact shear stress \( \sigma_{12} \) shows a gradient at the edges of the contact.

The corresponding horizontal displacement in Fig. 5.2c shows that some slip occurs during flattening, as a result of the lateral expansion of the asperity. The area over which slip occurs increases with decreasing friction coefficient. The contact with \( \mu = 0.7 \) does not slip during flattening, while for the two smaller fric-

\(^1\)http://www.engineeringtoolbox.com/friction-coefficients-d_778.html
tion coefficients slip has initiated from both sides of the contact (as to be expected in a Cattaneo-Mindlin problem).

5.3.2. DD results

In DD simulations, dislocations can nucleate and glide in the asperity and in a region below the asperity of dimensions $L_{pl} = 60 \mu m$ and $H_{pl} = 15 \mu m$ as shown in Fig. 5.1. Figure 5.3 shows that after yield the contact pressure increases very slowly with increasing displacement. The dislocation density, however increases rapidly to sustain the required plastic deformation. The dislocation density produced during flattening plays a key role during subsequent tangential loading for two reasons. First, there may be dislocations available to glide at a lower applied shear stress than the nucleation strength, so as to facilitate plastic shearing. Second, when dislocations are in the proximity of the contact, local slip may be induced by their fields.

Even though the contact is always under compression during elastic flattening, the presence of dislocations in the vicinity of the contact may locally induce a state of tension, and the contact detaches locally from the platen.

Comparison of the stress profiles predicted by the DD simulations in Fig. 5.4a and b with the corresponding elastic simulations in Fig. 5.2a and b reveals that the presence of dislocations in the vicinity of the contact gives rise to large stress fluctuations even though the contact area is continuous.

Figure 5.4c shows the horizontal displacement for different friction coefficients. By comparing the results of the DD simulations in Fig. 5.4c with the elastic results
5.4. Tangential loading of the asperity

AFTER FLATTENING TO $u_0 = 0.012 \mu m$ (cf. Fig. 5.2 and 5.4), or even further to $u_2 = 0.02 \mu m$, the asperity is loaded tangentially to $u_1 = 0.03 \mu m$.

5.4.1. Elastic results

Elastic simulations are performed for three friction coefficients, i.e. $\mu = 0.1$, 0.4 and 0.7. Figure 5.5 shows the contact shear stress normalized by the mean contact pressure $P_m$ during tangential loading versus the horizontal displacement of the platen, after flattening to $u_2 = 0.0012 \mu m$ and $u_2 = 0.02 \mu m$. For the smaller flattening depth, the contact slips completely for both friction coefficients, as attested by the plateau of the curves. When the flattening depth is larger and therefore the applied normal load is larger, full slip occurs only for the smaller friction coefficient.

For the smaller flattening depth, Fig. 5.6a shows the difference between the applied displacement and the horizontal displacement of the contact at the end of loading, when $u_1 = 0.03 \mu m$. It is found that for the smaller friction coefficients the contact has fully slipped at a rather small applied displacement, since the relative slip of the contacting surfaces is close to $0.03 \mu m$ everywhere. For the largest friction coefficient, sliding occurs much later.

Figure 5.4: The stress profiles (a) $\sigma_{22}$, (b) $\sigma_{12}$ and (c) the horizontal displacement of the contact, at the final flattening depth $u_2 = 0.012 \mu m$ for different friction coefficients.
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\[ \mu = 0.02 \]
\[ \mu = 0.0012 \]
\[ \nu_1 (\mu m) \]
\[ \tau /P_m \]
\[ 0 \ 0.01 \ 0.02 \ 0.03 \]
\[ 0.2 \ 0.4 \ 0.6 \ 0.8 \ 1 \ 1.2 \]
\[ \mu = 0.1 \]
\[ \mu = 0.7 \]

Figure 5.5: The contact shear stress normalized by the mean contact pressure for the asperity with \( w = 4 \mu m \) after flattening to different flattening depths.

\[ \Delta u_1 (\mu m) \]
\[ \sigma_{22} (\text{MPa}) \]
\[ \sigma_{12} (\text{MPa}) \]
\[ -2 \ -1 \ 0 \ 1 \ 2 \]
\[ -100 \ 0 \ 100 \ 200 \ 300 \ 400 \]
\[ \mu = 0.1 \]
\[ \mu = 0.7 \]

Figure 5.6: Elasticity: (a) the difference between the applied displacement and the horizontal displacement of the contact, (b) the \( \sigma_{22} \) and (c) \( \sigma_{12} \) profiles at the horizontal displacement \( u_z = 0.03 \mu m \) for different contact conditions. Prior to shearing, the asperity was flattened to \( u_z = 0.012 \mu m \).

Notice that when the friction coefficient is as small as 0.1, the surface is entirely under compression, as shown in Fig. 5.6b, while for a large value of the friction coefficient, \( \mu = 0.7 \), the stress at the right hand corner of the contact is set to zero, otherwise it would be under tension. Detachment in normal direction of the side of the contact results in a decrease of contact area of about \( 0.8 \mu m \) at the end of loading (see Fig. 5.6b), and a vanishing shear stress in the same region (see Fig. 5.6c).

5.4.2. DD results

In this section the asperity is tangentially loaded after being flattened to different depths with two different friction coefficients, \( \mu = 0.4 \) and \( \mu = 0.7 \). Results
in terms of mean contact shear stress, $\tau = \frac{F_y}{w}$ divided by mean contact pressure, $P_m = \frac{F_n}{w}$, are shown in Fig. 5.7; this ratio defines the macroscopic friction coefficient.

For a small flattening depth and therefore low contact pressure, the asperities behave elastically for both friction coefficients, and therefore macroscopic sliding occurs fully by slip of the contact. With increasing flattening depth (contact pressure), the plastic behavior becomes dominant for small shearing displacement (see Fig. 5.7a), but full slip of the contact finally occurs. Here, a contact is considered to be fully slipping when $|\langle \tau/P_m \rangle - \mu| \leq \mu \times 0.03$, where $\langle \tau/P_m \rangle$ is the average value of $\tau/P_m$ between $u_1 = 0.025$ and $u_1 = 0.03$. The value 0.03 is chosen to include wiggly curves like the blue one in Fig. 5.7a which have reached a plateau on average. Only for $\mu = 0.7$, see Fig. 5.7b, for the two largest flattening depth loading up to $u_1 = 0.03\mu m$ does not lead to de-adhesion of the contact and is fully accommodated by plasticity. Thus, the larger the contact pressure and the larger the friction coefficient, the larger the role played by plasticity. Notice that in Fig. 5.7b the curves for larger flattening depth do not start from zero, since during flattening dislocations were nucleated and therefore the final flattening depth has a shear stress different from zero, and dependent on the dislocation distribution.

Similarly to Fig. 5.6, Fig. 5.8 shows the relative displacement of the contacting surfaces and stress distribution for the intermediate flattening depth, $u_2 = 0.012\mu m$. Most importantly Fig. 5.8a reveals that slip of the contact with $\mu = 0.7$ is negligible, therefore the frictional behavior is controlled by plasticity (note that, in
contrast, full slip has instead occurred for $\mu = 0.1$. The stress profiles in Fig. 5.8b and c present high peaks. These peaks have smaller magnitude than those observed in previous studies (Sun et al., 2012) for discontinuous contact areas, and are simply the signature of the presence of dislocations close to the contact.

Figure 5.8: Discrete dislocation plasticity: (a) the difference between the applied displacement and the horizontal displacement of the contact for various friction coefficients, (b) the $\sigma_{22}$ and (c) $\sigma_{12}$ profiles at the horizontal displacement $u_1 = 0.03 \mu m$ for $\mu = 0.4$ and $\mu = 0.7$.

It should be noted that since the contact cannot be under tension, it detaches and causes the contact shear stress to increase as a consequence of the reduction in contact area. The decrease in contact area as shown in Fig. 5.9 occurs stochastically from regions of the contact where dislocations impinge, and not from the right hand corner of the contact as occurred when the behavior is fully elastic (cf. Fig. 5.6b).

Figure 5.9: The variation of true contact area at the flattening depth $u_2 = 0.012 \mu m$.

The distribution of shear stress and of the dislocations at the end of tangential loading is presented in Fig. 5.10 for the cases $\mu = 0.1$ and $\mu = 0.7$. Even
the case with smaller friction coefficient, which ends with a fully slipped contact, has an appreciable density of dislocations, nucleated partly during flattening (not shown) and partly during tangential loading. The density is significantly larger in the crystal with the larger friction coefficient. A very large shear band runs across the asperity and partly into the crystal underneath. For this crystal, a high density of dislocations piling up at or near the contact results in high-stressed areas where the contact opens up (see Fig. 5.10c and d for the contact profiles), thus decreasing the total contact area (cf. Fig. 5.9). In the presence of dislocations, not only the contact pressure but also the shear stress is highly inhomogeneous along the contact, thus very localized slip takes place at stochastic locations along the contact. This results in continuous redistribution of stress along the contact during loading.

As observed in Fig. 5.10 the occurrence of dislocation plasticity in the asperity does not imply that the contact remains completely adhered during tangential loading. However, if dislocation plasticity is absent the contact certainly looses adhesion and slips. The red curve in Fig. 5.11 denotes for any value of the friction coefficient, the maximum contact pressure for which not a single dislocation was
nucleated during tangential loading; beyond this pressure, slip is accompanied by plastic deformation, varying from local incipient plasticity to complete plastic shearing. The data points are obtained in the following way: if for a given friction coefficient and contact pressure only one realization out of three leads to a nucleation event, the simulations for the other two realizations are repeated with a progressively larger friction coefficient, until all three realizations lead to a nucleation event. The data point represents the average friction coefficient, while the error bars denote the spread in friction coefficient.

The blue line in Fig. 5.11, instead, distinguishes between contacts that fully slip and contacts that only slip partially. We remind the reader that a contact is considered to slip fully when \(|\langle \tau/P_m \rangle - \mu| \leq \mu \times 0.03\), where \(\langle \tau/P_m \rangle\) is the average value of \(\tau/P_m\) between \(u_1 = 0.025\) and \(u_1 = 0.03\).

Data points on the dashed-dotted lines correspond to the data in Fig. 5.7 at \(u_1 = 0.03\mu m\). For \(\mu = 0.4\) two simulations are fully elastic (A and B) while in the others some plastic activity develops during tangential loading. For the larger friction coefficient, \(\mu = 0.7\), two of the cases (D and E) involve so much plastic flow of the asperity that only partial slipping of the contact takes place. As expected, the higher the friction coefficient the larger the contribution of plasticity. Above the blue line the contact behavior is controlled by plasticity, below the red line by slip and in between lines, plastic relaxation is not sufficient to prevent full slip from occurring. Notice also that the slope of the blue curve changes rather
5.4. Tangential loading of the asperity

abruptly at larger mean contact pressure. As shown in Fig. 5.3, after yield, an increase of the flattening depth only requires a slightly higher contact pressure, but significantly affects dislocation density. In this figure, at large $P_m$ a small increase of contact pressure corresponds indeed to a large increase of flattening depth and dislocation density, therefore to a significant change in the response upon tangential loading: the larger the availability of dislocations the more plastic flow during shearing, even at a very low friction coefficient.

**Size effects**

Simulations are performed for asperities with the same aspect ratio $h_p/w = 0.5$ but a smaller size $w = 0.8 \mu m$ to investigate a possible size dependent response. The asperity is flattened to different values of depths and then tangentially loaded up to $u_1 = 0.03 \mu m$.

Figure 5.12(a) compares the frictional behavior of two self-affine asperities of different size flattened to various depth. For a friction coefficient $\mu = 0.6$ it is not possible to see any appreciable size dependence. When the flattening depth is small, the frictional response is fully controlled by interfacial slip and when the flattening depth is larger, a first plastic response is followed by slip. The curve for $u_2 = 0.012 \mu m$ and $w = 4 \mu m$ shows a harder response towards the end of the simulation than the smaller asperity. It should be noticed, though, that flattening asperities of different size to the same depth requires a different contact pressure. This is the reason why there is no size dependent behavior for these small and large asperities. In order to reveal the size dependence, we compare the frictional behavior of self-similar asperities flattened to the same pressure (see Fig. 5.12(b)): the behavior of smaller asperities is controlled by interfacial slip, while larger asperities tend to deform plastically. The situation presented in Fig. 5.12(a) is important in relation to the frictional behavior of two surfaces with very different elastic properties: one very compliant, the other nearly rigid. The nearly rigid body flattens different sized asperities to the same depth. When both surfaces have a similar compliance, the response would be in between what presented in Fig. 5.12(a) and (b): there will be a size dependence, but smaller than observed in Fig. 5.12(b).

For a better comparison between small and large asperities, Fig. 5.13 shows a similar mechanism map as Fig. 5.11 but now for $w = 0.8 \mu m$. The border of incipient plasticity is shifted to larger pressures for smaller asperities. This size dependence is slightly more pronounced when the friction coefficient is small. Figure 5.13 also indicates where full slip of the contact occurs, and where the contact only partially slips. Like for plastic shearing, the size dependence is strongest
when the friction coefficient is small. Evidently, when the friction coefficient is small, plasticity does not sufficiently support plastic flow in the small asperities, due to source limitation, and this results in earlier interfacial slip.

The results presented so far are clearly dependent on the size of the asperity. Yet, there is another key length scale: the mean distance between dislocation sources.

Figure 5.14 shows the frictional behavior of an asperity flattened to \( u_2 = 0.012 \mu \text{m} \) for various densities of dislocation sources. As expected, the smaller the spacing
between sources the larger is the applied sliding displacement necessary to reach the critical friction coefficient, $\mu = 0.7$.

![Figure 5.14: $\tau/P_m$ versus horizontal displacement for different dislocation source spacing.](image)

### 5.5. Conclusions

Discrete dislocation plasticity simulations were performed to investigate the static frictional behavior of a rectangular asperity protruding from a large single crystal. The contact between the asperity and a rigid platen is modeled such that slip at any contact point occurs when the shear stress at that point exceeds the normal shear stress times a constant (microscopic) friction coefficient. The simulation results lead us to the following conclusions.

- The larger the flattening depth and the contact pressure, the larger the effect of plasticity during tangential loading. Depending on its extent, plastic deformation can delay or completely suppress full slip of the contact.

- The larger the local friction coefficient, the more the macroscopic frictional behavior is controlled by plasticity. When the local friction coefficient is large, sliding is accommodated through plastic flow. When the local friction coefficient is small, tangential loading generally leads to full slip of the contact. However, if the flattening depth is so large that a high dislocation density is present, slip of the contact is only partial even if the friction coefficient is small.

- In the presence of dislocations, the contact pressure and shear stress is highly inhomogeneous along the contact. As a consequence localized slip takes
place at stochastic locations along the contact. This is different from what is observed elastically (see also the Cattaneo-Mindlin problem) where slip always starts from the edges of the contact.

- When self-similar asperities of different size are flattened to the same depth, their overall friction behavior is the same. This is because at the same flattening depth, small asperities are subjected to a larger contact pressure, but, due to source limitation, this has induced approximately the same plastic activity.

Instead, when self-similar asperities of different size are flattened to the same contact pressure, plastic deformation dominates the behavior of large asperities, while contact slip dominates the behavior of small asperities.

Our results suggest that the frictional behavior of surfaces, i.e. to which extent contacting bodies slide at the interface, strongly depends on the amount of plasticity generated during contact loading. When a large dislocation density is produced during normal loading, interfacial slip is less likely to occur. Plastic deformation of small asperities is source limited, but they are usually subjected to a larger pressure than large asperities, since their area of contact is smaller. Consequently when real rough surfaces are brought into contact and tangentially loaded, small asperities are not expected to slide before larger asperities.

**References**


Summary and conclusions

The ultimate objective of this work is to gain a better understanding of the plastic behavior of rough metal surfaces under contact loading. Attention in this thesis focuses on the study of single and multiple asperities with micrometer scale dimensions, a scale at which plasticity is known to be size dependent. The asperities have very simple geometries, either rectangular or sinusoidal and they are pressed into contact with a rigid platen.

The analysis is performed using the discrete dislocation (DD) plasticity method, given its accuracy to describe microscale plasticity and its capability of predicting size effects. In DD, plasticity is modeled as the collective motions of discrete dislocations, which are modeled as line singularities in an otherwise isotropic linear elastic medium. The dislocation Burgers vector is the material length scale that allows to capture plasticity size effects.

In Chapter 2, simulations are performed to investigate the flattening of a sinusoidal surface, for different dimensions and shape of the sinusoid.

A size dependent response is found for asperities with the same amplitude-to-period ($A/w$) ratio. The smaller asperities are more difficult to deform plastically due to the limited dislocation density at the same strain.

It is observed that the mean contact pressure can reach values up to about 40 times the yield pressure, thus significantly higher than what is predicted by the classical plasticity theory. This is mainly caused by the fact that the area of intimate contact is discontinuous and therefore the distribution of contact pressure is highly non homogeneous. Smaller contact regions are characterized by a very high stress concentration.

The simulation results are rather insensitive to the contact conditions used, i.e. frictionless or sticking.

When flattening periodic sinusoidal waves, it is not possible to assess a possible size dependence related to the spacing between asperities, since decreasing asperity spacing also reduces asperity size. Therefore in Chapter 3, simulations are performed for the flattening of an array of equally spaced sinusoidal asperities. This allows to investigate the effect of plastic interaction between neighboring asperities on the contact pressure.
It is found that the mean contact pressure necessary to flatten closely spaced asperities is larger than that required to flatten widely separated asperities. The so-called asperity density effect is already present in purely elastic materials, and becomes more pronounced when plasticity is described by discrete dislocations.

The origin of the asperity density effect is found to be a combination of plastic strain gradients, dislocation limited plasticity and interaction between plastic zones.

In Chapter 4, simulations are performed to investigate the effect of flattening on the subsequent shearing behavior of a rectangular asperity protruding from a large single crystal. The shearing is applied after the pillar is flattened to different depths. In large asperities, i.e. a couple of square micrometers, the dislocations generated during flattening promote early plasticity upon shearing, i.e. the contact shear stress is reduced, when plastic deformation takes place upon flattening. However, 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.

The simulations are also performed for on multiple asperities to investigate the effect of spacing on their shearing behavior. It is found that closely spaced asperities are 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.

In Chapter 5, simulations are performed to investigate the static frictional behavior of a metal asperity on a large single crystal, in contact with a rigid platen. The focus of this chapter is on understanding the relative importance of plasticity and contact sliding in a single asperity at a scale where plasticity is size dependent.

Sliding of a contact point is taken to occur when the shear traction exceeds the normal traction at that point times a friction coefficient. Plasticity initiates through the nucleation of dislocations from Frank-Read sources in the metal and is modeled as the collective motion of edge dislocation.

Results show that at large contact pressures and friction coefficients, plasticity controls the frictional behavior of a single asperity. When self-similar asperities of different size are flattened to the same depth while loaded tangentially, there is no trace of a size effect in their frictional behavior. However, when they are submitted to the same contact pressure smaller asperities slide while larger asperities deform plastically.
Samenvatting en conclusies

Het uiteindelijke doel van dit werk is het verkrijgen van een beter begrip van het plastische gedrag van ruwe metaaloppervlakken in mechanisch contact. De focus ligt in dit proefschrift op de studie van systemen met enkele of meerdere oneffenheden (asperities) op micrometerschaal, een lengte-schaal waarop bekend is dat plasticiteit grootte-afhankelijk is. De geometrie van de asperities is eenvoudig, namelijk rechthoekig of sinusoïdaal, en de asperities zijn in contact met een onvervormbare plaat.

De analyse is uitgevoerd met de discrete-dislocatie (DD) plasticiteit-methode, die een nauwkeurigheid heeft die hem geschikt maakt voor het bestuderen van microschaal plasticiteit en die mogelijke grootte-afhankelijke effecten kan voorstellen. Plasticiteit is gemodelleerd als het collectieve gedrag van dislocaties, die gemodelleerd zijn als lijn-singulariteiten in een verder isotroop, lineair elastisch medium. De methode maakt gebruik van de Burgersvector van de dislocatie, die de materiaal-afhankelijke lengteschaal is van plasticiteit, waardoor hij in staat is om grootte-afhankelijke effecten in plastische deformaties te voorspellen.

Hoofdstuk 2 beschrijft simulaties uitgevoerd om het afvlakken van een sinusoïdaal oppervlak voor verschillende grootten en vormen te bestuderen.

Voor asperities met gelijke amplitude/periode-verhouding ($A/w$) is een grootte-afhankelijk gedrag gevonden. De kleinere asperities zijn moeilijker plastisch te deformeren, wat veroorzaakt wordt door de kleinere dislocatiedichtheid, bij dezelfde rek, dan bij grotere asperities.

De gemiddelde contactspanning kan oplopen tot circa 40 keer de vloei spanning, wat dus significant hoger is dan wat de klassieke plasticiteitstheorie voor spel. Dit wordt voornamelijk veroorzaakt doordat het contactoppervlak op microschaal discreet is en daardoor de verdeling van contactspanningen in hoge mate inhomogeen is. Kleinere contactgebieden worden gekarakteriseerd door zeer hoge spanningsconcentraties.

De resultaten van de simulaties zijn vrij ongevoelig voor de condities van het contact, zoals wrijvingsloos of perfect adhesief.

Bij het afvlakken van periodieke sinusoïdale profielen is het niet mogelijk om de eventuele invloed van de afstand tussen de asperities op het gedrag te analyseren, aangezien het verkleinen van die afstand ook de asperity zelf verkleint.
Daarom worden in Hoofdstuk 3 simulaties uitgevoerd voor het afvlakken van een rij asperities met gelijke tussenruimte. Hierdoor kan het effect van de plastische interactie tussen naburige asperities op de contactspanning bestudeerd worden.

De gemiddelde contactspanning die nodig is voor het afvlakken van asperities met kleine tussenruimte blijkt hoger te zijn dan voor asperities met grote tussenruimte. Dit zogenoemde asperity-dichtheidseffect is al aanwezig in puur elastische materialen en wordt versterkt door plasticiteit.

De oorsprong van het asperity-dichtheidseffect wordt gevonden in de combinatie van de plastische rekgradiënt, plasticiteit met een beperkt aantal dislocaties en de interactie tussen plastische gebieden.

In Hoofdstuk 4 zijn simulaties beschreven die gedaan zijn om het effect van afvlakken op het afschuifgedrag van rechthoekige asperities op een groot eenkristal te bestuderen. Het afschuiven is uitgevoerd voor pilaren die waren afgevlakt tot verschillende dieptes. In grote asperities, van enkele vierkante micrometers, induceren dislocaties, gegenereerd tijdens het afvlakken, vroege plasticiteit bij het afschuiven. De schuifspanning in het contact wordt gereduceerd wanneer plastische deformatie plaatsvindt tijdens het afvlakken. Het afvlakken van kleinere asperities tot dezelfde verplaatsing heeft echter geen effect op het daarna uitgevoerde afschuiven. Hoewel er veel dislocaties aanwezig zijn in de asperities, is de afstand tussen de dislocaties op een klein aantal actieve slipvlakken klein, waardoor de mobiliteit van de dislocaties laag is.

De simulaties zijn ook uitgevoerd voor systemen met meerdere asperities, om het effect van de tussenruimte tussen de asperities op het afschuifgedrag te bestuderen. Het blijkt dat een kleinere tussenruimte leidt tot een lagere schuifspanning dan die voor geïsoleerde asperities. Dit effect wordt voornamelijk veroorzaakt doordat het afschuiven van asperities met kleine tussenruimte in het elastische regime leidt tot een breed gebied direct onder de asperity waar de schuifspanning hoog is en daardoor nucleatie van dislocaties veroorzaakt. Dit effect verdwijnt wanneer de asperities hoog uitsteken boven het kristal en plasticiteit voornamelijk in de asperity zelf plaatsvindt.

De simulaties in Hoofdstuk 5 werden uitgevoerd om het statisch wrijvingsgedrag van een metalen asperity in contact met een onvervormbare plaat te bestuderen. De focus van dit hoofdstuk ligt op het begrip van het relatieve belang van plasticiteit en glijden in het contact zelf, op een lengte-schaal waarop plasticiteit grootte-afhankelijk is.

Een contactpunt gaat glijden wanneer de schuifkracht groter is dan de normale kracht op dat punt vermengvuldigd met een wrijvingscoëfficiënt. Plasticiteit wordt geïnitieerd door de nucleatie van dislocaties uit Frank-Read bronnen in
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het metaal en is gemodelleerd als het collectieve gedrag van edge dislocaties.

De resultaten laten zien dat voor hoge contactspanningen en wrijvingscoëfficiënten, plasticiteit dominant is in het wrijvingsgedrag van een enkelvoudige asperity. Wanneer gelijkvormige asperities met verschillende grootte worden afgevlakt tot dezelfde diepte tijdens het afschuiven, wordt er geen spoor van een grootte-effect in het wrijvingsgedrag waargenomen. Echter, kleinere asperities, met dezelfde contactspanning als grotere asperities, schuiven af in het contact, terwijl grotere asperities plastisch deformeren.
Acknowledgements

Since I came to Holland in 2009, it has been a relatively long time to finish this PhD thesis. I am grateful to my daily supervisor Dr. Lucia Nicola for her kind help and useful suggestions in the past years. I feel honored and pleasant to do this PhD project under her supervision. Her contribution of thorough analysis, sparkling ideas and critical comments makes my work fruitful. Modification of my paper definitely needed much patience of my supervisor’s that I appreciated. I would like to thank my promoter Prof. dr. Barend J. Thijsse, who shared with me some important tips on the structure of the thesis. During my tough period of searching a job, his suggestion on resume, experience in interview and encouragement are really helpful.

I am also very grateful to Prof. Erik van der Giessen from University of Groningen for his serious modification of my papers and helpful discussions in M2i cluster and progress meetings.

This research was carried out under project number MC 2.06282 in the framework of the Research Program of the Materials innovation institute (M2i) in the Netherlands (www.M2i.nl). I would like to thank the financial support from M2I and the industrial partners Tata steel and Daf Trucks. I would also like to express my appreciation to Matthijs Toose, Henk Vegter from Tata steel, Johan Zijp and Nico Kamperman from Daf for their critical comments and kind suggestions in every progress meeting.

I would like to extend my appreciation to my colleagues Yunhe Zhang, Robbert-Jan Dikken, Kelvin Wei Siang Ng and Astrid Gubbels-Elzas for helpful discussions which happened to inspired me with new ideas. My special thanks to Robbert-Jan, Astrid and Barend for their translation of my thesis into Dutch. I would also like to thank my previous promoter Prof. Ian Richardson for his suggestions on how to do a successful research. Sincere thanks to the secretaries Anneke van Veen and Anke Kerklaan-Koene.

I want to thank Chuangxin Zhao, Guiming, Song, Yu Pan, Sepideh Ghodrat, He Gao, Murugaiyan Amirthalingam, Vera Popovich, Xi Zhang, Weichen Mao, Qing-shi Song, Yingxia Qu, Zhiguang Huan and Xueqing Zhang for their warm and friendly help.
Last but not least; I would like to thank my parents and my wife Ju for their understanding, support, and patience in my life.
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