Influence of tip adhesion on nanoindentation and scratching

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Abstract
Using molecular dynamics simulation, we study the influence of tip adhesion on nanoindentation and scratching. By using a model pair potential between tip atoms and substrate atoms, we can arbitrarily change the adhesion strength. For the prototypical case of a diamond tip and a bcc Fe substrate, we find that with increasing adhesion strength, the indentation hardness and also the normal hardness during scratching decreases. Even more pronounced is a strong increase of the transverse force and hence of the friction coefficient during scratching. The indent pit becomes atomically rough, and the pileup produced during scratch increases with increasing adhesion strength. On the other hand, the length of the dislocations produced and the spatial extent of the plastic zone shrinks.

Keywords: molecular dynamics, nanoscratching, pile-up, iron, dislocations, plasticity, hardness

1. Introduction
Molecular dynamics (MD) simulations of nanoindentation are usually performed with a repulsive indenter [1, 2]. There are several reasons for this choice. (i) The repulsive interaction is the mandatory part to convey forces from the tip to the substrate in order to remove atoms and form an indent pit or a scratch groove. (ii) The often-employed non-atomistic
indenter introduced by Kelchner et al. [3] is best motivated for a purely repulsive force field between indenter and substrate. (iii) The realistic inclusion of attractive forces between indenter and substrate requires a knowledge of the (surface) chemistry between the two solids, which may be highly complex. (iv) In reality, indenter tips and substrate surfaces will be covered by (unknown) adsorbate layers which diminish the attraction between the pure materials. Rather than including the adsorbate layers into the model, the simulation is simplified by the choice of an (effective) repulsive tip-substrate potential.

We note that a number of nanoindentation simulation studies exist which do use an attractive interaction potential. These are often concerned with the chemical effects induced. Thus, early work [4] indeed used an adhesive tip for modeling Ni-tip indentation into a Au substrate and showed the consequences of decorating the tip with substrate atoms as well as forming a neck between the tip and the substrate during tip retraction. More recently, the effects of surface chemistry on the tip-substrate interaction during contact were investigated for the special case of a C tip approaching a Ni surface [5]. The differences between indenting a clean, a hydrogenated, and an oxidized surface were studied using MD simulations with particular emphasis on the mass transfer between the tip and the substrate. Stoyanov et al. [6] studied the interaction of a hydrogenated diamond-like carbon (a-C:H) asperity with a tungsten surface in order to understand the mechanical and chemical processes occurring during a sliding process. By using a bond-order potential developed by Justlin et al. [7] for the W-C-H system, they studied both the processes occurring in W and in the a-C:H specimen. Transfer of W to the a-C:H surface and H diffusion into W were observed, while transfer of C was not reported.

The inclusion of attractive interactions into the modeling also allows to study the tool wear during indentation. For example, Narulkar et al. [8] use the Lee potential [9] to study graphitization of the diamond tool during machining of an Fe workpiece; to this end they describe the C–C interaction by using the Tersoff potential [10] in order to describe the diamond-graphite phase transformation faithfully.

However, only few studies exist up to now which investigate the influence of the tip-substrate potential on the results of indentation [11–13]. In the present paper, we study the effect of an attractive tip-substrate potential on nanoindentation and scratching simulations. We choose a model interaction potential between tip atoms and substrate atoms that allows us to switch on the attractive part arbitrarily and choose its strength. This allows us to identify the effects that attraction induces to the forces felt by the indenter, the hardness of the substrate measured during the process, the plasticity developed in the substrate and the topography of the groove and pileup, among others. We deliberately exclude the effects of chemistry between tip and substrate and the issue of tool wear and focus on the effects of tip adhesion on the substrate.

2. Method

2.1. Simulation method

The substrate consists of a single-crystalline block of Fe with a (100) surface. We introduce a cartesian axis system, in which \( z \) (along [100]) is normal to the surface, while \( x \) ([011]) and \( y \) ([0\overline{1}1]) lie in the surface plane. The simulation volume has extensions of 75.1, 85.2 and 61.5 nm in \( x \), \( y \) and \( z \) direction, and consists of \( 22.1 \times 10^6 \) atoms. After relaxation of the Fe crystal, two atomic layers at the bottom and the lateral sides are fixed to prevent the workpiece from any translational or rotational movement during indentation and scratch. The next four layers are kept at a temperature of 1 mK by a velocity-scaling thermostat. Fe atoms
interact via the Mendeleev potential (number 2) [14]; this potential has a cut-off radius of 5.4 Å.

The tip is modeled as an atomistic sphere (radius $R = 10$ nm) cut out from a block of diamond. The tip is considered to be rigid; i.e. all C atoms have fixed distances to each other during the simulation such that no C–C interaction potential needs be applied, since the motion of C atoms is described by kinematics rather than by forces. The interaction between C and Fe atoms is described in detail in section 2.2 below.

The tip is initially positioned at 5.6 Å above the surface, i.e. immediately outside the C–Fe interaction. For the indentation simulation the indenter moves into the substrate up to the final depth of $d = 4$ nm; then it is retracted. The contact radius for full indentation is given by

$$a_c = \sqrt{R^2 - (R - d)^2},$$

and amounts to $a_c = 8$ nm. The scratch simulations start from the fully indented position; then the tip moves in the (011) direction up to the total scratch length of 15 nm and is finally retracted. In all stages, the indenter velocity amounts to 20 m s$^{-1}$.

The scratch direction was chosen such that the prominent (111) glide systems in bcc Fe produce slip both along the scratch direction as well as perpendicular to it, i.e. to laterally to the sides of the grooves. The simulation volume was large enough to enclose all dislocations generated.

We use the open-source LAMMPS code [15] with a constant time step of 1 fs to perform the simulations. The dislocation extraction algorithm (DXA) [16] is used to identify the dislocations, to determine their Burgers vectors, and to measure the total length of the dislocation lines, $L_{\text{dis}}$. The free software tools ParaView [17] and OVITO [18] are employed to visualize the atomistic configurations.

### 2.2. Adhesive model potential

The study of the interaction of Fe and C has a long tradition, and a multitude of interaction potentials have been developed to describe the interaction of Fe and C atoms in bulk materials. We mention pair potentials [19, 20] and many-body potentials [9, 21–28] to describe the interaction of interstitial C in Fe, potentials for carbides [24, 26–29] and for mixed Fe–C clusters [30]. In the present study, however, we will base our description on a simple pair potential approach. This is motivated by the model character of our study, which aims at understanding the consequences of an adhesive in contrast to a repulsive tip on indentation and scratching.

We are inspired by the work Gao et al [31] on the wetting of C nanotubes and graphene sheets by Fe. They use a Lennard-Jones (LJ) potential

$$\Phi_{\text{LJ}}(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^6 - \left( \frac{\sigma}{r} \right)^2 \right]$$

with a well depth $\epsilon = 94.63$ meV, and a length parameter $\sigma = 2.05$ Å, leading to an equilibrium Fe–C bond length of $r_0 = 2.30$ Å. These parameters are based on ab-initio work by Durgun et al [32] on the interaction of a single Fe atom with a C nanotube, and differ somewhat from an alternative, but less well founded, approach by Banerjee et al [33].

We wish to keep the force during the repulsive part of this interaction ($r < r_0$) identical to this potential equation (2), since it determines the way how the tip will remove Fe atoms during indentation and scratching. However, we want to fix the well depth of the potential to an arbitrary value $-D$. The adhesive part ($r > r_0$) is then modeled such that the potential smoothly goes to zero at a cut-off radius $r_c$; we choose $r_c = 5.4$ Å, as in the Fe–Fe potential [14]. We
therefore use the following potential

\[
\Phi(r) = \begin{cases} 
-2D \left[ \frac{(r - r_0)}{(r_c - r_0)} \right]^3 - 3 \left( \frac{r - r_0}{r_c - r_0} \right)^2 + 1, & r_0 < r \leq r_c, \\
0, & r > r_c.
\end{cases}
\] (3)

The third-order spline in the region \(r_0 < r \leq r_c\) guarantees continuity of the energy and force at \(r = r_0\) and \(r = r_c\).

We denote the free parameter of this potential, \(D\), as the strength of the adhesion; we shall use \(D/\epsilon = 0, 0.5, 1\) and 2. While \(D = 1.0\epsilon\) corresponds to the realistic parameter value [31], we also use smaller and larger values in order to see the effect of adhesion more clearly. The potential is plotted in figure 1 for the adhesion strengths used in this paper.

3. Indentation

3.1. Forces and hardness

Figure 2(a) shows the basic information of an indentation simulation, viz. the load–depth curve. As usual, this figure combines the force during the indentation part and the retraction part of the tip trajectory; the indentation part is characterized by larger forces. A strong influence of the adhesive forces can be observed. These influence in particular the retraction part of the tip trajectory. The substrate that has obtained close contact with the tip exerts strong bonding forces to the tip. Also the position where the tip loses contact to the substrate changes from 25 Å (for the repulsive tip) to 20 Å for \(D = 0.5\epsilon\) and even to around 10 Å for the more strongly adhesive tips. In the case of the strongest adhesion, \(D = 2.0\epsilon\), strong force fluctuations show up on the retracting trajectory that extend to distances above the surface;
they demonstrate that an atomistic contact between the tip and the Fe atoms persists for a long time during the retraction phase.

But also during the penetration part of the indentation, effects of adhesion are observed. While the tip is still above the surface—at negative indentation depths in figure 2(a)—the adhesive interaction leads to negative forces, which drag the tip towards the surface. Further on during the entire penetrating part of the trajectory, the loading force is smaller for more strongly adhesive tips; this demonstrates that adhesion drags the tip into the substrate and hence assists the loading force.

By dividing the pressure by the contact area (projected onto the surface plane), the instantaneous contact pressure can be calculated, see figure 2(b). Initially—before the indenter reaches the surface and also in the first 5 Å after penetrating the surface—the contact pressure assumes quite large negative values, as adhesion drags the tip towards the surface. Then the pressure increases with depth. Beyond an indentation depth of around 25 Å the contact pressure stabilizes. The average value of the contact pressure is denoted as the material hardness, since it describes the pressure that has to be exerted on the material to induce permanent plastic deformation. In our case we take the average over the last 20 Å of indentation. In order to differentiate this hardness value from other hardness values that describe the material response during scratch, we denote the hardness calculated during indentation as the indentation hardness $H_{\text{ind}}$. The values of $H_{\text{ind}}$ are tabulated in table 1. Hardness decreases with increasing adhesion $D$ for the same reason that the indentation force decreases. For the case of strongest adhesion, $D = 2.0\varepsilon$, the reduction in hardness becomes particularly pronounced.

### 3.2. Plasticity and topography of the pit

Indentation produces dislocation plasticity in the material; for the case of bcc materials in general [1, 2, 34] and Fe in particular [35], the dislocation network has been well studied by atomistic simulations. Dislocations with Burgers vector $\mathbf{b} = \frac{1}{3}(111)$ and $(100)$ are created, which form a dense network adhering to the indent pit. Remington et al [36] discuss in detail the nucleation of plasticity and the emission of dislocation loops during indentation of bcc materials. They point out that shear loops are generated in the region of highest shear stress under the indenter; these loops expand with leading dislocation lines of an edge character followed by trailing lines of a screw character. Only upon further indenter penetration, and
Table 1. Characteristics of the plastic zone after full indentation and after tip retraction. Data are for various adhesion strengths, $D$.

|       | $D = 0$ | $D = 0.5\epsilon$ | $D = 1.0\epsilon$ | $D = 2.0\epsilon$ |
|-------|---------|--------------------|--------------------|--------------------|
| Indent | Retraction | Indent | Retraction | Indent | Retraction | Indent | Retraction |
| $L_{\text{disl}}$ (nm) | 874 | 557 | 800 | 404 | 895 | 336 | 905 | 335 |
| $R_{\text{pl}}$ (nm) | 32.2 | 25.0 | 30.8 | 21.3 | 28.1 | 23.8 | 27.6 | 23.7 |
| $f$ | 4.03 | 3.13 | 3.85 | 2.66 | 3.51 | 2.98 | 3.45 | 2.96 |
| $H_{\text{ind}}$ (GPa) | 17.15 | 16.24 | 16.21 | 14.50 |

Notes. $L_{\text{disl}}$: total dislocation length within plastic zone. $R_{\text{pl}}$: size of plastic zone. $f$: plastic-zone size factor. $H_{\text{ind}}$: indentation hardness.
concomitant loop expansion, do the trailing screw lines annihilate leading to a pinch-off of the shear loop and its emission as a prismatic loop. In consequence, emission of prismatic dislocation loops is only observed for larger penetration depths \([1, 34, 37]\), but not in the cases studied here, as our indentation depth of 4nm is too shallow. We display in figure 3 the dislocation structures that have formed below the indent pit. While the largest extension of the network is clearly for the case of the repulsive tip, no drastic changes in the network can be read off this figure.

We quantify the dislocation network by the total length of dislocation lines, \(L_{\text{disl}}\), and by the radius of the plastic zone, \(R_{\text{pl}}\). In the case of dislocation plasticity, \(R_{\text{pl}}\) can be defined as the largest distance of a dislocation segment from the center of the contact area (projected into the surface plane) \([37]\). From theoretical considerations \([38]\), but also from experiment \([39]\), it is known that \(R_{\text{pl}}\) scales with the contact radius \(a_c\), equation (1), such that it is advantageous to introduce the plastic-zone size factor as

\[
f = \frac{R_{\text{pl}}}{a_c}.
\]

We assemble these data in table 1. During the indentation process, the length of the dislocation network does not show a clear trend but rather fluctuates between 800 and 905 nm for the different tips studied. This is understandable, since the length of the dislocation network is connected to the size of the indent pit; according to the theory of geometrically necessary dislocations \([40]\), a certain number of dislocations are necessary to remove the material from the pit, and hence \(L_{\text{disl}}\) does only marginally depend on the force field used and hence not on the adhesive properties of the tip. On the other hand, the size of the network, \(R_{\text{pl}}\), shows a clear trend of smaller values for higher adhesion. This is understandable from the fact

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**Figure 3.** Dislocation network after retraction of the indenter. Dislocations are colored according to their Burgers vector \(b\): blue \(\frac{1}{2}(111)\), red (100). Yellow denotes the surface of the indent pit as well as unidentified defects. Data are for various adhesion strengths, \(D\).
that for higher adhesion, smaller indentation forces are needed; consequently also the stress fields in the substrate are smaller and these do not expand the dislocations as much as larger stress fields do.

During tip retraction, of course the network recedes, decreasing $R_{pl}$, and it simplifies by contracting shear loops and by the annihilation of dislocations on the surface of the indent pit, decreasing $L_{disl}$. After retraction, the data in table 1 show that the plastic-zone radius is largest for the repulsive tip; however, the values for the various adhesive tips are not very different from each other and from the repulsive tip. This feature is corroborated by the snapshots shown in figure 3, where the variation in the internal structure of the dislocation network appear to be larger than the variations in the outer extension of the network. The plastic-zone size factor $f$ assumes values of 3 or slightly below; this is in line with other simulation studies [37].

The total length of the network, $L_{disl}$, shows a clearer trend in that it decreases with increasing adhesion $D$. This effect is particularly pronounced for the repulsive tip, where the large shear loops extending in lateral direction—connected to the large plastic-zone radius—appear to be responsible for the large value of $L_{disl}$.

The indent pit after retraction of the indenter is shown in figure 4. For the repulsive tip, we observe a rather smooth wall of the pit, in which some faceting caused by the crystalline order of the material is still seen. The pileup of material emitted on top of the surface is also visible. While the topography only slightly changes for the case of the weakest adhesion, $D = 0.5\epsilon$, for larger adhesion strengths, $D = 1.0\epsilon$ and $D = 2.0\epsilon$, a strong roughening of the excavated pit becomes apparent. This roughness is caused by substrate material bonded to the tip, see figure 7 below, where the tip is shown after scratching; upon retraction of the tip, these atoms leave the pit together with the tip. A bridge forms between the substrate and Fe atoms bonded to the tip which eventually ruptures rendering the pit surface rough, while some substrate material adheres to the surface.
During scratching, we have to differentiate between the normal force $F_n$ necessary to keep the tip at the predetermined depth of $d = 4$ nm, and the tangential force $F_t$ which moves the tip at this depth along the surface. These forces are plotted in figures 5(a) and (b), respectively. Both forces feature an onset regime of around 3–4 nm, in which the normal force drops as the rear part of the moving tip loses contact to the substrate, while the tangential force builds up.
from its initially vanishing value. The normal force then stays roughly constant, apart from fluctuations, while the tangential force features a slightly increasing trend, as the forming frontal pile-up offers additional resistance to the moving tip.

The normal force decreases with increasing adhesion for the same reason as during indentation: the adhesive component of the force helps keeping the tip at its level. Note, however, that the effect is more pronounced than for the case of indentation, figure 2(a). The tangential force shows an even stronger change upon adhesion as it strongly increases from around 1 to 2 μN with increasing adhesion. This increase is caused by the shell of substrate atoms bonded to the tip that augment its transverse area and thus enlarge the resistance of the material against tip motion.

Both for the normal force and the transverse force, fluctuations increase with $D$. The bonds induced by the attractive forces between tip and substrate atoms leads to stick-slip behavior which becomes apparent in the force fluctuations. Here, stick-slip describes the phenomenon that the scratch tip does not slide smoothly over the surface; rather, because of adhesion—or in other cases, because of rough surface topography—the tip repeatedly sticks to the surface, and then slips. This results in a non-steady tip motion giving rise to strong force fluctuations. Such a behavior has been seen previously both in experiments and in dedicated MD simulations [41–44].

Again the determination of the contact areas is important for quantifying the contact pressures. For scratching, a normal and a transverse contact area are needed which give the contact area projected onto the surface plane and onto a plane normal to the scratch direction. The determination of these contact areas is not without subtleties. In macroscopic experiments, it is reasoned that the contact areas can be determined from the geometry of the tip [45]. The normal contact area is assumed to be of semicircular form

$$A_{\text{norm}}^{\text{geo}} = \frac{1}{2} \pi a^2,$$

as the rear half of the tip loses contact with the substrate during scratch. The transverse contact area is assumed to be equal to the lateral projection of the submersed part of the tip; it has the geometrical form of a circular segment with area

$$A_{\text{trans}}^{\text{geo}} = \frac{1}{2} R^2 [2\theta - \sin(2\theta)].$$

Here, $\theta$ is the semi-angle at the center of the spherical tip subtended by the groove,

$$\cos \theta = \frac{R - d}{R}.$$

For our geometry these areas amount to $A_{\text{norm}}^{\text{geo}} = 100.5 \text{ nm}^2$ and $A_{\text{trans}}^{\text{geo}} = 44.7 \text{ nm}^2$.

In an atomistic simulation, we are able to determine the atoms that are in contact with the tip and infer from these the contact areas; details of the procedure are provided in [46]. The main idea here is that a distance criterion decides whether a substrate atom is in contact with the tip; a summation over the (projected) areas of these atoms then gives the total contact area. Since the area is provided by the atoms surrounding the tip, it is slightly larger than the geometric area of the tip. For the case of indentation with its clearcut geometry, the geometrical normal tip area amounts to 201 nm$^2$, while the atomistic method gives 227 nm$^2$.

Figures 5(c) and (d) show the evolution of the contact areas with scratching as evaluated with the atomistic method. The normal contact area of the repulsive tip drops from its initial value of 225 nm$^2$ to an average value of 170 nm$^2$; a decrease of only 24% rather than 50% as assumed in the macroscopic estimate, equation (5). This is caused by the fact that for nanoscopic tip sizes, also part of the rear surface touches the groove bottom, see [46]. With
increasing adhesion strength, an increasingly larger fraction of the total semicircular tip area is in contact with the substrate; already for \( D = 1.0 \), after the full scratching length of 15 nm, the contact area amounts to the equivalent of a full circle, 226 nm\(^2\). For the largest adhesion, \( D = 2.0 \), the normal contact area increases monotonically during the entire scratch. As shown in figure 8, this is caused by substrate atoms bound to the tip above the surface. However, these atoms will not transmit forces between the tip and the substrate as they are high above the substrate surface. We must therefore conclude that the atomistic method of determining the contact area here encounters problems. The transverse contact area, figure 5(d), steadily increases in all cases; this is caused by the pileup produced. Even a weak adhesion strongly changes the growth rate of the transverse contact area, as it allow substrate atoms to become (permanently) attached to the tip. Initially, upon indentation, the transverse contact area is in good agreement with the geometrical estimate, equation (6), but exceeds it later strongly due to the growing pileup. The macroscopic estimate does not take this pileup into account.

From the forces and the areas, we may determine the contact pressure, figures 5(e) and (f). Its values, averaged over the last 5 nm, give us the normal and transverse hardness; their values are assembled in table 2, where also the hardness values as calculated from the geometrical areas are added. The normal contact pressure shows a strong decrease with increasing adhesion. This is partly due to the decreasing normal force, and hence also persists for the geometrical normal hardness. Since in addition also the normal contact area increases with adhesion, the atomistically calculated hardness is strongly below the geometrical hardness. As noted above, the calculation of contact areas is no longer reliable in cases of (strong) adhesion.

The transverse contact pressure shows a non-monotonic behavior in that it first strongly increases in the onset regime; later during steady scratching it saturates (for the repulsive tip) or even decreases (for the adhesive tips). The decrease for the adhesive tips is caused by the growing pileup and in particular the strong increase of substrate atoms bonded to the tip. As table 2 shows, the atomistically calculated transverse hardness is rather independent of the attraction strength. The geometrically calculated hardness, on the other hand, rises strongly with adhesion and assumes unrealistically high values; this is caused by the complete neglect of the contribution of the pileup to determining the transverse contact area.

We conclude that while the determination of the forces acting on the tip is trivial in MD, the determination of the contact pressure is not, since the evaluation of the pertinent contact areas is complicated. For a repulsive tip there are good arguments that atoms that are in contact with the tip (based on a distance criterion) will also contribute to convey forces between tip and substrate and can therefore be used to estimate the contact area. For an adhesive tip, however, substrate atoms may be bound to the tip without conveying forces to the substrate; these are irrelevant for determining the contact area. We take this as a warning that the determination of contact pressures in simulations using adhesive tips is nontrivial.

We finally determine the friction coefficient

\[
\mu = \frac{F_t}{F_n},
\]

in figure 6; since it is based on forces only, its determination is straightforward. Averages over the last 5 nm are provided in table 2. The friction coefficient strongly increases with adhesion; this is mainly due to the strong increase of the transverse forces, figure 5(b). Note the large fluctuations in the case of strong adhesion which originate from the transverse-force fluctuations, figure 2(b), caused by the stick-slip behavior showing up in the case of adhesive forces.
| $D$ | $L_{disl}$ (nm) | $R_{pl}$ (nm) | $f$ | $H_{norm}$ (GPa) | $H_{trans}$ (GPa) | $H_{norm geo}$ (GPa) | $H_{trans geo}$ (GPa) | $\mu$ |
|-----|----------------|---------------|-----|-----------------|-------------------|---------------------|----------------------|-----|
| 0   | 1457           | 1240          | 4.31| 12.15           | 13.63             | 21.61               | 26.64                | 0.57|
| 0.5e| 1464           | 1241          | 2.70| 10.16           | 10.92             | 20.38               | 32.30                | 0.70|
| 1.0e| 1275           | 771           | 2.93| 8.37            | 12.39             | 18.39               | 37.22                | 0.94|
| 2.0e| 1185           | 804           | 3.10| 5.89            | 13.44             | 17.37               | 41.65                | 1.11|

**Notes.** $L_{disl}$: total dislocation length within plastic zone, including emitted loops. $R_{pl}$: size of plastic zone. $f$: plastic-zone size factor. $H_{norm}$: normal hardness. $H_{trans}$: transverse hardness. $H_{norm geo}$ ($H_{trans geo}$): normal (transverse) hardness calculated from a geometrical approximation of the contact area. $H_{trans geo}$: transverse hardness. $\mu$: friction coefficient.
We note that macroscopic experiments are well described by assuming that the friction coefficient is given by

\[ \mu_{\text{geo}} = \frac{A_{\text{geo}}}{A_{\text{norm}}} \]  

This estimate is based on the assumption that normal and transverse hardness coincide. For our geometry, this prediction gives \( \mu_{\text{geo}} = 0.45 \), in fair agreement with the simulation result for the repulsive tip immediately after the onset regime (scratching length around 4 nm); with increasing scratch length, of course, the simulated friction coefficient rises due to the frontal pileup which requires more and more transverse force for scratching. A good agreement of the macroscopic law equation (9) with nanoscopic MD simulation results has already previously been noted [47].

4.2. Plasticity and pileup

The dislocation plasticity generated below the scratch grooves is displayed in figure 7; the lengths of the dislocation networks generated are assembled in table 2. We observe that under scratching, dislocation loops are emitted. As in the case of indentation, we see that the length of the dislocation network formed decreases with increasing adhesion. This decrease is already visible in the plasticity after full scratch before retracting the tip and is exacerbated after retraction. Note that while the tip continues scratching, the rear part of the groove is already unloaded and the dislocation network below it may relax. This relaxation process provides for the reason why already the fully scratched groove shows a considerable influence of tip adhesion on the dislocation length, while indentation did not.

The grooves scratched with a strongly adhesive tip \( (D = 1.0\sigma \text{ and } D = 2.0\sigma) \) have a by one third reduced dislocation activity. As in the case of indentation, this is caused by the reduced normal force needed to scratch with the adhesive tip.

The radius of the plastic zone, \( R_{\text{pl}} \), is determined here as the lateral distance of the farthest dislocation segment from the groove axis [48], since the length of the plastic zone along the axis is essentially determined by the scratch length. We see that plastic-zone radii correspond
Figure 7. Dislocation network after scratching and retraction of the tip. Dislocations are colored as in figure 3. Data are for various adhesion strengths, $D$. 
to those determined under indentation; again a reduction of $R_{pl}$, with increasing adhesion is observed which is caused by the smaller normal forces.

Finally, figure 8 displays the pile-up formed after the tip has been retracted from the groove. Note that even a small adhesion, $D = 0.5\varepsilon$, leads to a strong height increase of the pileup; part of the pileup is bonded to the tip and is moved with it upwards during retraction. In the cases of stronger adhesion, $D = 1.0\varepsilon$ and $D = 2.0\varepsilon$, substrate atoms are also bonded laterally to the tip.

5. Summary

Tip adhesion to the substrate leads to a number of changes as compared to a purely repulsive tip.

1. In indentation, the effects are subtle. The indentation force is slightly decreased by the attractive part of the interaction such that also the indentation hardness is slightly reduced. In consequence the dislocation network below the indenter shrinks both in radial expansion and in total length. The indent groove becomes atomically rough as during withdrawal of the tip after indentation some wall atoms adhere to the tip surface and are removed from the pit.

2. In scratching, the effects are more pronounced. As the pileup will adhere to the tip, the transverse force during scratching substantially increases and so does the friction coefficient. This effect is even magnified by a reduction of the normal force, which is similar in origin but more pronounced in magnitude than for indentation. Also in scratching the dislocation network below the scratch groove shrinks for an adhesive pit.

From a methodological point of view, the calculation of the load-bearing contact areas in normal and transverse direction becomes difficult for an attractive tip since not all parts of the tip that are in contact with substrate material transfer forces.

While the present study focuses on the effects of adhesion of substrate material to the tip, in a real machining situation, chemistry will also influence the tip itself. The effects of tool
wear, while certainly relevant in experiment and application, have been little studied in simulations [5, 49] and further studies into this effect would be welcome.

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