Single-asperity contributions to multi-asperity wear simulated with molecular dynamics

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Abstract. We use a molecular dynamics approach to simulate the wear of a rough ferrite surface due to multiple hard, abrasive particles under variation of normal pressure, grinding direction, and particle geometry. By employing a clustering algorithm that incorporates some knowledge about the grinding process such as the main grinding direction, we can break down the total wear volume into contributions from the individual abrasive particles in a time-resolved fashion. The resulting analysis of the simulated grinding process allows statements on wear particle generation, distribution, and stability depending on the initial topography, the grinding angle, the normal pressure, as well as the abrasive shape and orientation with respect to the surface.

1. Introduction
Most molecular dynamics (MD) simulations treat two-body wear as a nanometric cutting process and focus on the interaction between a single abrasive particle and a usually flat substrate [1, 2, 3]. However, wear processes may involve circumstances such as changing rough topographies, random abrasive orientation distributions or wear debris build-up between neighbouring abrasives, which cannot be studied using the above approach. The implementation of a statistically based surface roughness in an MD model combined with multiple abrasive particles acting on the surface is therefore useful for more realistic modelling of wear phenomena [4, 5, 6, 7]. In this way, the interactions between abrasives/asperities are explicitly included in the model, while the results, if properly evaluated, retain most of the information from the single-asperity level.

In this work, we simulate the abrasion process of an atomically rough ferrite surface with 16 hard abrasive particles implicitly bonded into a matrix using MD. By dynamically identifying the atoms which are worn away from the substrate, the wear volume can be quantified and monitored in a time-resolved fashion. Moreover, every nanoscopic wear particle is affiliated with the abrasive particle by which it is produced using an iterative clustering algorithm. This allows a thorough analysis of the individual contributions of the abrasive particles to the wear volume. We describe our MD model as well as the simulation procedure in section 2, where we also give a short summary of how the clustering algorithm identifies the wear particles. In section 3 we first briefly present some exemplary worn topographies, followed by a more in-depth discussion of the time dependence as well as the distribution of the individual abrasive contributions to the wear volume, based on two selected examples. We also bring up two special cases, eventually showing...
the limits of the clustering algorithm. We conclude with a listing of five major influences on wear particle stability in section 4.

2. Computational details

2.1. Model

Our single-crystal ferrite substrate has lateral dimensions of $28.5 \times 28.5 \text{ nm}^2$, an initial average height of 28 monolayers, and exposes a (001) surface to the abrasives. Its periodically replicated topography features a near-Gaussian height distribution with a root mean squared roughness of 0.78 nm, an arithmetic mean height of 3.94 nm, a nominal asperity width of 2 nm, and a maximum random lateral asperity site offset from the regular grid of 1 nm, see figure 1. More information on the topography generation procedure can be found in [4]. At the substrate base, three rigid monolayers of Fe atoms form support, covered by two monolayers that are kept at a temperature of 300 K. This is done via a Langevin thermostat acting only in $y$ direction so that it does not overly interfere with the movement of the abrasive particles and the applied pressure. The abrasive particles are modelled as rigid bodies arranged in a staggered $4 \times 4$ grid as shown in figure 1, rotated randomly between 0 and 90 degrees about all three Cartesian axes, and they are initially placed several nanometres above the surface. Two abrasive particle geometries are considered: spherical with a radius of $3.25 \text{ nm}$ and cubic with a side length of $4.2 \text{ nm}$, chosen to provide a high degree of surface coverage without allowing overlap between neighbouring abrasives. A state-of-the-art Finnis-Sinclair potential is used for the Fe–Fe interactions [8], while the interactions between abrasive particles and the substrate is modelled using a Lennard-Jones potential with the parameters $\varepsilon = 0.125 \text{ eV}$ and $\sigma = 0.2203 \text{ nm}$. These values are comparable to [2, 9, 10, 11] and yield an interaction roughly one order of magnitude weaker than the one for Fe–Fe, leading to mild adhesion.

![Figure 1](image_url)

**Figure 1.** Top view of the initial substrate topography coloured according to local height (red is high, blue is low). The numbered outlines of the 16 spherical (left) and cubic (right) abrasives in their initial positions are superimposed with individual rainbow-style colouring for future reference. Note that abrasives #8 and #16 straddle a simulation box boundary. Below, the four grinding angles $\alpha$ are schematically shown.
2.2. Simulation procedure
All wear simulations were performed using the open-source MD code LAMMPS [12]. We apply periodic boundary conditions in the $x$ and $y$ directions, meaning that if an atom leaves the simulation box through one boundary, it re-enters at the opposing one. The abrasive particles are dragged across the surface at a sliding velocity in $x$ direction of $v^{(\text{max})} = 16$ m/s at four different angles $\alpha$ of $\pm 7.1^\circ$ and $\pm 3.6^\circ$ with the $x$-axis, so that the abrasives re-enter the simulation box at different $y$ positions every time they pass the periodic box boundaries and therefore do not immediately follow in their own grinding marks, see the lower part of figure 1. Since the $y$ component thus introduced increases the total sliding velocity by less than 1\%, only the $x$ component is discussed henceforth. The particle positions relative to each other are locked throughout the simulations, and particle rotation is not allowed as would be the case for a grindstone. Furthermore, the particles cannot change their $z$ positions individually depending on the topography, but only collectively. This leads to occasional loss of surface contact for individual abrasive particles for some time intervals, while the remaining particles share the increased load. The abrasive particles themselves are not subject to any wear. The normal pressure $\sigma_n$ on the abrasives is kept constant at values of 0.1, 0.5, and 1.0 GPa for the entire simulation time of 15 ns, corresponding to a total abrasive translation of $\Delta x = 240$ nm. It therefore takes a given abrasive 1.8 ns to perform one sweep of the entire simulation box.

The $x$ component of the Fe atom velocities, $v = v_x$, is Gauss-filtered with a total filtering window of 0.4 ns and a standard deviation of 0.2 ns to yield the pure atomic drift velocities without any thermal contribution. Atoms with a momentary drift velocity of $v > 0.9 v^{(\text{max})}$ are considered wear particles, those essentially at rest with $|v| < 0.1 v^{(\text{max})}$ are part of the substrate, while all remaining atoms that do not belong to the abrasive particles are currently under shear [4]. The number of atoms in the wear particles can then be multiplied with a per-atom volume of 11.6 Å$^3$, leading to a wear volume $V_w(t)$ equivalent to the wear depth $h_w(t)$ defined in [6].

2.3. Identification of individual wear particles
As discussed in further detail with respect to contact zones in [4], it is possible to clusterize the contributions of the individual abrasives to the total wear volume $V_w(t)$ by iteratively searching for wear particle atoms which lie closer than $d_{\text{clus}} = 0.4$ nm to abrasive particles or other wear particle atoms whose abrasive affiliation is already known. The number of affiliated wear particle atoms may stop growing due to problems arising from the periodic boundary conditions, namely unaffiliated atoms with their affiliated neighbors at the other side of the simulation cell. This can be solved by once mapping all atoms in question which lie closer than $d_{\text{clus}}$ to the lower cell boundary across the upper cell boundary. Thus for the next iteration, a sufficient number of affiliated atoms is available on the correct side of the cell boundary so that further affiliations can be made. Finally, single outliers and small groups of outlying atoms join the closest clusters with known affiliation. This last step introduces a small error to the break-down of the total wear volume, as isolated wear particles without a single initial particle affiliation may be falsely affiliated with close yet unrelated abrasives in this way. The above method works very well for non-coalescent wear particles. As the build-up of wear debris between two abrasives at higher normal pressures becomes sufficient to form a single uninterrupted wear particle, it becomes a matter of definition which part of that particle should be identified with a given abrasive. Our algorithm initially searches for affiliated atoms only in sliding direction, which largely hinders the iterative “backwards growth” of abrasive affiliation observed in coalescing wear particles.

3. Results and Discussion
In figure 2, we give the reader an idea of what the final surfaces, including the wear particles, look like after grinding at different normal pressures. While some features from the original topography remain visible as blue areas for the lowest normal pressures (left), the other
topographies are dominated by the geometries of the abrasive particles. It is also obvious from the comparison of the images in the right column that cubic abrasives produce larger wear particles by way of cutting, which also have a tendency to coalesce, while spherical abrasives produce smaller, more evenly distributed wear particles that result mainly from ploughing.

Figure 2. Exemplary final topographies after grinding at normal pressures of 0.1, 0.5, and 1.0 GPa (from left to right) with spherical abrasives (top) or cubic abrasives (bottom). The surface atoms are coloured according to their local height, where blue denotes valleys, yellow is the original mean height, elevated parts are shown in green and the extreme tips in red. The grinding angle was $\alpha = -3.6^\circ$ in both examples.

We discuss the individual abrasive contributions to the total wear volume by means of some examples shown in figure 3. There we selected two examples of what we consider (based on the large body of available load- and grinding-angle-resolved data) two typical cases as well as two special cases that require separate discussion. In the left panel of each row, we show the time development of the total wear volume broken down into the individual abrasive contributions, coloured according to the abrasive key colour scheme introduced in figure 1 and used throughout this contribution. This representation allows the tracking of the emergence, stability, and possible destruction of wear particles as well as the occurrence of periodic phenomena. The center column in figure 3 shows a side-by-side comparison of time-averaged wear volume contributions with error bars representing the time variance over the entire grinding duration. This bar chart layout lends itself well to study emerging patterns which might be explained with the initial topography, the normal pressure, the grinding angle, the asperity shape or orientation. Finally, on the right, we have included a top-view snapshot of the wear particles only, coloured according to their abrasive affiliation. This allows us to check how well the clustering algorithm determined abrasive affiliations and how it handled wear particle coalescence. It also allows us to estimate the order of magnitude of the error made when a wear particle is in physical contact with more than the one abrasive that produced it, thus leading to a number of false affiliations.

Rows 1 and 2 in figure 3 represent typical results at a normal pressure of 0.5 GPa for spherical and cubic abrasives, respectively. It is obvious that the cubic abrasives produce more than
Figure 3. Left column: time dependent break-down of wear volume with respect to abrasive particle; centre column: comparison of time-averaged per-abrasive wear volumes; right column: top view of distribution and affiliation of wear particles at $t = 15$ ns. Rows from top to bottom: (1) spherical abrasives at 0.5 GPa, $\alpha = -7.1^\circ$, (2) cubic abrasives at 0.5 GPa, $\alpha = +3.6^\circ$, (3) spherical abrasives at 0.1 GPa, $\alpha = -7.1^\circ$, (4) cubic abrasives at 1.0 GPa, $\alpha = -3.6^\circ$. 
three times as much wear as the spherical abrasives. However, when breaking the wear volume down into individual abrasive contributions, it becomes clear that while spherical abrasives can produce wear particles with an average volume of $\approx 10 \text{ nm}^3$, only three out of 16 do so. A comparison of row 1 with figure 1 explains why abrasives #5 and #8 immediately produce sizeable wear particles at a grinding angle of $\alpha = -7.1^\circ$, as two large asperities of the initial topography lie directly on their respective trajectories. When looking at the time-dependent representation at the left of row 1, we see that wear particles #6 and #7 are formed after $\approx 1.5 \text{ ns}$ and then remain stable, while the smaller wear particle #3 is re-incorporated into the substrate after 5 ns.

By contrast, ten out of the 16 cubic abrasives produce similarly sized or even larger wear particles, see row 2 in figure 3. Of the remaining six, abrasives #2, #3, and #8 have disadvantageous orientations for producing large wear particles (see figure 1), as they do not present a cutting edge to the surface, and they also hardly come into substrate contact at this intermediate normal pressure. The two neighbouring abrasives #15/#16 have somewhat “complementary” orientations so that their ability to produce wear particles depends greatly on the grinding angle, with abrasive #16 favouring positive grinding angles and #15 negative ones. The same applies, to a lesser extent, to abrasives #9/#10. A comparison of the wear volume time development between rows 1 and 2 shows that the wear particles produced by cubic abrasives, once formed, are more stable over time than those formed by spherical abrasives.

Row 3 in figure 3 represents a special case of grinding with spherical abrasives at low normal pressure, a process characterized by small wear volumes, unstable wear particles, as well as an initial peak/plateau of the total wear volume that subsides after 2.5–5 ns (when the roughness has reached its minimum), followed by a small, constant residual wear volume. The only two (stable) wear particles worth mentioning in the example shown in row 3 of figure 3 are #5 and #13, both of which are formed at the very beginning of the process due to the positions of their abrasives with respect to the initial asperities.

The second special case is presented in row 4 of figure 3. Here the top-view snapshot of the wear particles coloured according to their abrasive affiliation exhibits several examples of possibly false affiliation. At high normal pressure, cubic abrasives can form such large wear particles that some of them may touch the abrasive preceding them, which leads to false affiliation of several atoms. However, the error introduced to the break-down of the total wear volume in this way is small compared to the size of the wear particles. By contrast, wear particle coalescence, as seen between wear particles #12 and #15, as well as #4, #7, and #8, may present a greater challenge. Here, the general question arises how to correctly determine which part of a large wear particle was caused by which abrasive.

Taking into account the grinding angle of $\alpha = -3.6^\circ$, it seems obvious for a human observer that a sizeable portion of what the clustering algorithm considers wear particle #12 should actually be considered a part of wear particle #15. Likewise, much of wear particle #4 is produced by abrasives #7 and #8. While the clustering algorithm employs some of the information (such as the main grinding direction) available to a knowledge-based analysis, it is currently unable to decide that, e.g., a wear particle is unlikely to be produced by the trailing edge of an abrasive. The implementation of such complex considerations into the algorithm is the focus of ongoing work.

The onset of false affiliations cannot be linked to specific threshold values such as the total wear volumes or the normal pressure. In fact it is a combined effect of the load, the initial topography, the size correlation between abrasives and asperity shapes and well as grinding direction relative to topographic features. Therefore the illustrations of the wear particle affiliations in the right column of figure 3 prove to be the best indicator for the limitations of a chosen simulation parameter set. Note, however, that a slightly incorrect particle affiliation does not influence the total wear volume. In contrast to our “dry” simulations under vacuum conditions, even
in presence of a medium (e.g., O$_2$ or a lubricant), the same atoms would form wear particles, though possibly with some interface layers or free surfaces.

The false affiliations, however, are not the cause for the wear volume oscillations that can be seen in the left panel of row 4. These are rather the result of a large wear particle breaking off to the side, being re-incorporated into the substrate, and then being picked up by one of the following abrasives. Such oscillations only occurred for cubic abrasives at high normal pressures and negative grinding angles and seem to be connected with coalescing wear particles, as these have a higher likelihood of re-incorporation into the substrate between two abrasives.

**Figure 4.** Break-down of the mean wear volume into individual abrasive contributions for spherical abrasives (a) and cubic abrasives (b), grouped by normal pressure. Grinding angle $\alpha$ within each group (from left to right): $+7.1^\circ$, $+3.6^\circ$, $-3.6^\circ$, $-7.1^\circ$.

In figure 4 we summarize the individual abrasive contributions to the total wear volume for all our simulations. The time-averaged particle-resolved wear volumes are displayed as stacked bars coloured according to abrasive affiliation and arranged in a way that allows the analysis of the dependence on the normal pressure as well as the grinding angle. The left panel shows the results for spherical abrasives and the right one those for cubic abrasives. We observe that the total wear volume is almost grinding-angle independent for cubic abrasives at low to intermediate normal pressures (varying only by approximately 3%), while the relative spread of the data produced by spherical abrasives is roughly ten times as high. At 1.0 GPa, the total wear volume varies by about 10%, depending on the grinding direction, for both abrasive geometries, and this dependence seems somewhat correlated between the two shapes. This serves as an indicator that at this normal pressure the orientation of the individual abrasives has little overall influence on the wear volume. Finally, the representation of the data in figure 4 also shows that, independent of normal pressure, the distribution of wear particles among the abrasives is much more stable with respect to varying grinding angles for cubic abrasives.

4. **Summary and Conclusion**

We have employed a recently proposed and partly knowledge-based clustering algorithm to break down the total wear volume occurring in nanoscopic grinding simulations into contributions of the individual abrasive particles. Based on the above, we can conclude that the stability of individual wear particles is influenced by:

(i) The initial position of the abrasive with respect to the original topography as well as the grinding angle. If the first topographic feature an abrasive encounters on its path upon
striking the surface is a pronounced asperity, it will quickly produce a relatively large wear particle.

(ii) Existence of deep pits along the trajectory of the wear-particle-producing abrasive. Especially if these pits are encountered soon after the first wear particle has formed, there is a high chance that a large portion of the wear particle will be re-incorporated into the substrate there.

(iii) Abrasive shape. Spherical abrasives do not exhibit any large surfaces consisting of crystallographic planes, so wear debris attached to them can be more easily sheared off than from the cubic abrasives, which exhibit bcc (100) planes.

(iv) Abrasive orientation. While almost irrelevant for spherical abrasives, orientation is of high importance for the cubic abrasives as it and the grinding angle determine the rake angle, depending on which a given abrasive will tend more towards cutting or ploughing. Certain orientations (e.g., crystallographic planes nearly parallel to the surface) may even rule out appreciable wear particle formation except at the highest normal pressures.

(v) Wear particle detachment. Fortuitous detachment of a wear particle from the surface may prevent subsequent re-incorporation into the substrate and thus leads to a perfectly stable wear particle.

Our multi-asperity MD simulations have the advantage over single-asperity simulations that they can reflect the interactions between wear particles produced by individual abrasives in real grinding processes (and partly also wear processes). This could be shown by the wear particle affiliations and the sensitivity study with respect to the grinding angle. Compared to other simulation techniques (e.g., FEM), we believe that MD combined with proper surface topography analysis techniques is a suitable tool for describing real grinding processes at the nano-scale.

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