Plastic activity in nanoscratch molecular dynamics simulations of pure aluminium

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Abstract:

Aiming at a better understanding of the atomic origins of friction in crystalline metals, a simple friction case - single-asperity nano-scale scratching of aluminium - is simulated in molecular dynamics (MD). MD and atomistic models in general suffer from strong length- and time-scale limitations and one needs to be very careful to avoid the creation of non-physical phenomena due to too small simulation boxes and too high rates. In order to investigate how the simulation size (substrate thickness and scratching depth) and rate (scratching speed) influence the resulting friction mechanisms, a large parametric study has been performed in which substrate thickness, indentation depth and scratch speed have each been varied for more than an order of magnitude. The general set-up of the simulations can be seen in Figure 1. Both single-crystal and nano-crystalline substrates have been considered. The rigid spherical indenter has a radius of 23 Å, which is about an order of magnitude smaller than a typical atom force microscope probe tip.
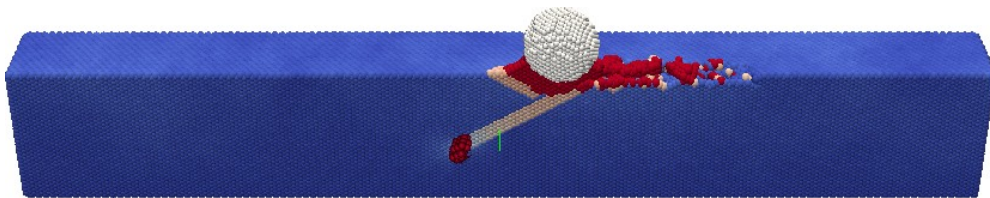
Figure 1: Snapshot during simulation: white atoms belong to the rigid indenter, the red atoms in the centre surround a dislocation loop. Only half of the simulated domain is shown in order to make the plastic deformation in the bulk under the indenter and in the groove behind the indenter visible.

A regression-based method to compute the friction coefficient μ based on measurements extracted from the simulation is presented as well as a statistically motivated criterion to determine whether differences in friction coefficients are statistically significant. Furthermore, a clean way to separate the scratching work into heat production Q and variation of stored plastic energy E_{pl} using molecular dynamics combined with molecular statics is derived. Figure 2 shows

a comparison between dislocation activity and the evolution of E_{pl}. The excellent fit between the evolutions of these two quantities indicates that E_{pl} is indeed a good measure for the energy stored in plastic zones.
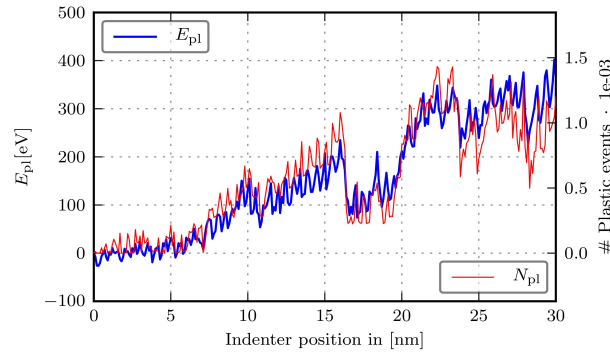

Figure 2: Comparison between plastic energy E_{pl} and plastic count N_{pl}. Both plots share the abscissa. The values of E_{pl} (heavy line) are to be read on the left ordinate, the ones of N_{pl} (light line) on the right ordinate. The good agreement between the two curves suggests that E_{pl} is a good measure for the energy stored in plastic zones.

We demonstrate that in order to understand how the simulation parameters influence the results, it is not sufficient to analyse the sensitivity of μ, because both Q and E_{pl} remain size and rate dependent even in size and rate ranges in which μ appears to have stabilised.

When comparing single-crystal and nano-crystalline substrates, the evolution of E_{pl} reveals fundamentally different friction mechanisms for these two cases. While the single crystal substrates always accumulate plastic energy during scratching, the nano-crystalline substrates actually *release* energy during scratching by relaxing and recrystallising their micro-structure near the surface.

We observe that both Q and E_{pl} are rate dependent over the entire range of scratch speeds considered in this study. However, while the amount of heat Q generated over one scratch increases with increasing scratch speed, E_{pl} shows the opposite trend. Over the range of investigated substrate thicknesses, Q becomes size independent for the larger substrates, but the plastic energy remains size sensitive. This indicates that the plastic zones are not resolved, even for the relatively small scratch case covered in this parametric study.