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Plastic activity in nanoscratch molecular dynamics simulations of pure aluminium

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ABSTRACT

Atomistic models for friction suffer from the severe length- and time-scale restrictions of molecular dynamics. In this paper, a novel approach to quantify the scratching work and the energy associated with plastic activity is used. The approach is combined with a statistical criterion to determine the significance of simulation box size, microstructure and sliding rate effects on the friction coefficient. This method is applied to a large parametric molecular dynamics study of single-asperity nanoscratch on monocrystalline and polycrystalline aluminium substrates. The results show that even though simulation size affects the plastic core mechanisms of sliding friction, the method overcomes size dependence when it comes to the predicted value of the friction coefficient. We show that friction in monocrystalline and polycrystalline substrates activates very different mechanisms and describe them in some detail for the polycrystalline case. Furthermore, we show that even when the friction coefficient appears to be size independent over a range of simulation box sizes, the plastic activity associated with it remains non-monotonically size dependent.

1. Introduction

Traditionally, tribology has been the study of macro-scale contact and has been dominated by experiments (Amontons, 1699; Rabinowicz, 1995; Blau, 2008). One goal of tribology is to predict friction, i.e. the friction coefficient, from material properties and contact topology. There are two main sources of challenges preventing prediction. On one hand, contact as a mechanics problem involves all length scales, from atomistics to the scale of the structure, and therefore all time scales from the period of atomistic vibrations to the duration of contact. On the other hand, it involves complex mechanisms such as third body interactions, plasticity, frictional heating and melting. At the same time, the push towards surface effect dominated micro- and nano-electromechanical systems as well as the use of atomic force microscopy (Giessibl and Jul, 2003) make it more important to understand mechanical contact at its fundamental scale, the single-asperity nano-scale contact.

Luan and Robbins (2005) showed that nano-scale contact is ruled by atomistic phenomena and virtually always accompanied by plastic deformation in the form of dislocation nucleation at the surface or asperity flattening (Luan and Robbins, 2009). With the exception of simple cases, such as nano indentation (Engels et al., 2012), these phenomena cannot be captured or understood using continuum mechanics because of their inherently discrete nature. Discrete dislocation dynamics (Bulatov and Cai, 2006) studies attempt to solve this problem by modelling the motion of individual dislocation loops but do not offer accurate treatment of dislocation nucleation, which has been shown to be an important factor (Nicola et al., 2007,

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2008). On the other hand, molecular dynamics (MD) naturally handles both dislocation motion and nucleation (Bulatov and Cai, 2006; Griebel et al., 2007). There have been many MD studies of nano-scale contact. While the early ones suffered more from the inherent length and time scale restrictions of MD (e.g., Komanduri et al., 2000), modern computing hardware allows for the investigation of more and more realistic contact cases (Szlufarska et al., 2008). Relevant studies include the investigation of the influence of indenter sizes and shapes (Nair et al., 2008; Gao et al., 2009; Chandross et al., 2008), of surface roughness (Spijker et al., 2011, in press), indentation depth and third bodies (Liu and Szlufarska, 2010), surface chemistry (Mo and Szlufarska, 2010; Mo et al., 2009; Brukman et al., 2006), nano-machining (Romero et al., 2012) and surface coating (Liu et al., 2012). However, to the best of our knowledge, there has not been a systematic quantitative investigation of the degree to which the plastic mechanisms involved in friction contribute to the overall friction and how they depend on simulation parameters such as simulation box size, sliding speed and microstructure, even though plasticity in frictional contact determines wear and tear.

Non-continuum analytical models exist, but they usually involve perfect flat on flat contact and are based on the assumption that interfaces are considerably weaker than bulk material (e.g. Merkle and Marks, 2007).

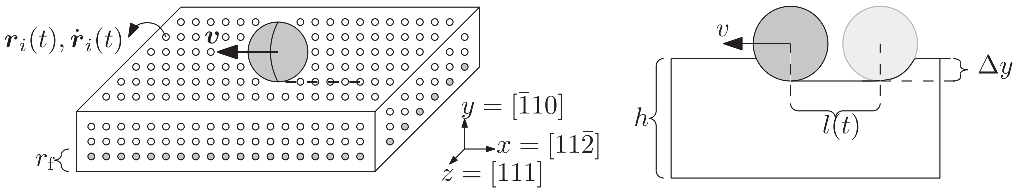
We present a novel molecular dynamics based method to quantify the energies associated with the creation of plastic zones during friction. In continuum plasticity theory, separating the work of thermomechanical processes into energetic and dissipative plastic contributions based on thermodynamic considerations is well established and its validity experimentally confirmed (Mróz and Oliferuk, 2002). Usually, the energetic contribution is attributed to the energy stored in dislocation networks and the dissipative contribution to dislocation motion (Voyiadjis and Faghihi, 2012). There is an ongoing discussion on how to model these two phenomena at the continuum scale, see Voyiadjis and Faghihi (2012) for a thorough presentation.

Our method allows to perform this separation of work at the atomistic scale without a priori assumptions. We apply it to a parametric study of single asperity nano-scale scratching of a crystalline aluminium substrate. Aluminium has been chosen as an application example, but the presented method is suitable for any crystalline metal. The simulation setup and parameter space are presented in Section 2. Section 3 derives the details of the method from the molecular dynamics energy balance. The study investigates the influence of scratching speed, substrate thickness, indentation depth and microstructure. The results are presented in Section 4, where we also show a fundamental difference between friction mechanisms in polycrystalline and monocrystalline substrates.

2. Molecular dynamics setup

2.1. Single crystal case

The scratching simulations included in this paper combine molecular dynamics (MD) simulations with molecular statics (MS) minimisations and have the same basic setup, shown in Fig. 1(a). The system is composed of a rigid spherical indenter and a deformable block-shaped substrate. Most of the parametric study deals with single crystal substrates. Both indenter and substrate are modelled by aluminium atoms governed by the Mendelev embedded atom model (EAM) potential (Mendelev et al., 2008) of the form



(a) Schematic simulation setup: Grey atoms in the bottom layer represent fixed atoms within r_f from the bottom boundary. The velocity vector $\boldsymbol{v}$ is imposed on all indenter atoms, $\boldsymbol{r}_i(t)$ and $\dot{\boldsymbol{r}}_i(t)$ are the position and velocity vectors of atom i. The crystal orientation of both the indenter and the substrate with respect to the coordinate system is shown in Miller indices.

(b) Schematic depiction of scratch parameters; h is the substrate thickness, Δy the indentation depth. The scratch speed v is applied by imposing the indenter position $l(t) = vt$ at time t.

Fig. 1. (a) Schematic simulation setup: Grey atoms in the bottom layer represent fixed atoms within r_f from the bottom boundary. The velocity vector $\vec{v}$ is imposed on all indenter atoms, $\vec{r}_i(t)$ and $\dot{\vec{r}}_i(t)$ are the position and velocity vectors of atom *i*. The crystal orientation of both the indenter and the substrate with respect to the coordinate system is shown in Miller indices. (b) Schematic depiction of scratch parameters; *h* is the substrate thickness, Δy the indentation depth. The scratch speed v is applied by imposing the indenter position $l(t) = vt$ at time *t*.