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Nanoscratching of iron: A molecular dynamics study of the influence of surface orientation and scratching direction

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ABSTRACT

Using molecular dynamics simulation we study scratching of Fe crystals by a hard repulsive tip. Three surface orientations – (100), (110), and (111) – are studied with two scratch directions in each case. We take care to analyze the projected normal and transverse contact areas properly to take the loss of contact of the tip to the substrate beneath it and its increased contact to the pile-up into account. We find that the form of the pile-up generated depends strongly on the surface orientation and scratch direction; this dependence is analyzed with the help of the dominant slip system in bcc Fe. The normal force to keep the tip at fixed depth and the transverse scratching force vary by only 15% between the different scratch systems investigated. The normal contact area decreases considerably during the initial stage of scratching as the trailing part of the tip loses contact with the substrate. The normal hardness shows similarly small variations between the different systems studied and is smaller than the hardness during the indentation process. The transverse contact area increases continuously during the scratch as the pile-up is generated. As a consequence the tangential hardness varies more strongly (by 26%) between the systems studied. For the (100)[011] scratch system we analyze the depth dependence of scratching. We find the friction coefficient to increase with scratch depth. The dependence of the normal and tangential hardness on depth are discussed with the help of the variation of the respective projected areas with depth.

1. Introduction

The scratching of a surface by a hard tip, which is indented into the surface, is a standard method to determine the lateral mechanic response of a substrate [1]. Sometimes this method is denoted as 'ploughing' [2] in order to differentiate it from sliding experiments where the tip stays above the surface [3].

During scratching, two different hardness values are often introduced in tribological research [4] to characterize the materials response. The first measures the response of the material to the normal force, and will be termed *normal hardness*, H_{norm}, while the response to the tangential (or lateral) force will be denoted as the *tangential hardness*, H_{tang}. The first hardness value is similar in concept to the hardness determined in indentation simulations; in order to distinguish these two quantities the terms *(static) indentation hardness* (determined by indentation) and *scratch hardness* (determined by scratching) are often used. The tangential hardness is also denoted as the *ploughing hardness* [5,6].

We note that in early studies indentation and scratch hardness were considered to exhibit numerically equal values, with the argument that both characterize the resistance of the material to plastic deformation, and their size must therefore be determined by the critical plastic flow pressure of the material [7,8]. Later work found that the two hardness measures need not coincide, in particular not in single crystals where crystalline anisotropy affects the plastic response [9–11]. Also it may be expected that due to the different loading conditions in indentation and scratch – in particular the different contributions of shear – the two hardness values can differ from each other.

Experimentally, hardness is determined as the quotient of the applied forces and the contact areas. The determination of the contact areas is not without uncertainties. During scratching, it is not clear which part of the indenter still has contact with the substrate beneath, and what is the amount of the pile-up generated during scratch that contribute to the transverse contact area. Simulation offers the possibility to determine the relevant areas unambiguously at every instant of time during scratch [12]; thus

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the determination of both normal and tangential hardness is possible in simulation.

Szlufarska et al. [13] give an up-to-date account of experimental and theoretical advances in sliding contacts. Gouldstone et al. [14] review advances in the field of indentation and compare experimental and simulational scales. Junge and Molinari [15] discuss plastic activity in scratching Al single- and polycrystals; they focus on separating the contributions of potential energy created by dislocation generation from energy dissipation by dislocation motion.

The processes occurring in bcc metals due to the indentation process have been studied in detail by molecular-dynamics simulation. Defect generation and pile-up of atoms during nanoindentation of Fe single crystals was described by Smith et al. [16] and later by Lu et al. [17]. The nanoindentation contact of a W tip in W was studied by Hagelaar et al. [18]. Defect nucleation and evolution in Ta nanoindentation was investigated by Biener et al. [19] and by Alcalá et al. [20]. This work was continued by Ruestes et al. [21] who performed a detailed indentation study into Ta, and investigated the influence of indenter radius, penetration velocity, and interatomic potentials on defect creation and evolution. Gao et al. [22] characterized the plastic zone created by nanoindentation in Ta and Fe, and compared it with the plastic zones created in fcc metals, Al and Cu.

A number of nanoscratching simulations have been performed in recent years. The majority of these studied the response of fcc metals such as Cu, Al or Au [2,23–28]. As to scratching of bcc metals, the only previous studies have been performed for Fe substrates. We mention Mulliah et al. [2], who discuss the depth dependence of the friction coefficient, Lu et al. [29] who use a triangular prismatic indenter, and our previous study [30] which focuses on the analysis of the evolution of the dislocation network during scratching. However, the indentation process has been studied repeatedly for bcc metals; simulation works include studies of W [18], Ta [19–21] and Fe [16,17,31–33].

In this paper we study the consequences of scratching a prototypical bcc material, α-Fe. Section 3 focuses on the dependence of scratching on the surface orientation and the scratching direction. These influence primarily the formation of the pile-up generated above the surface and the dislocation pattern below the surface. In addition the friction coefficients and the normal and tangential hardness, which provide a quantitative measure of the scratch process, will be determined. For the calculation of the hardness coefficients, a careful determination of the contact areas – both normal to the load and normal to the scratch direction – are required; their calculation is discussed in Appendix A. The depth dependence of the scratching process is studied – for a single selected scratch system in Section 4. Finally we assess the temperature dependence of our simulations by comparing simulations performed at 300 K with those at 0 K, Appendix B.

2. Simulation method

We study nanoscratching of Fe single crystals by using the technique of molecular-dynamics (MD) simulation. The simulation system is depicted schematically in Fig. 1, in which the configuration of the spherical nanoindenter and the Fe substrate are shown. The simulation proceeds in three steps: (i) the indenter is pushed along the $-z$ direction into the substrate (indentation); (ii) the indenter moves along the x direction at the indentation depth (scratching); (iii) the indenter is moved out of the substrate to return to its initial height above the surface (retraction).

The scratching tip is composed of 7248 C atoms arranged in a rigid diamond lattice structure. It has a spherical shape with a radius of $R = 21.4$ Å. As substrates, we use bcc Fe single crystals

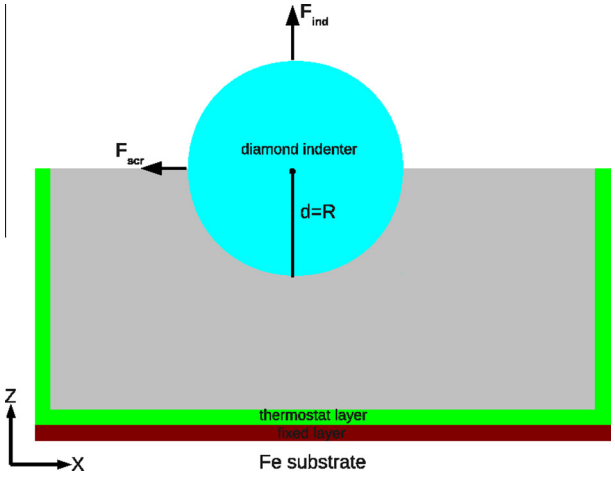

Fig. 1. Setup of the scratching system. The indentation depth d is equal the radius of the indenter R. The normal force F_{ind} and scratching force F_{scr} are shown. The substrate has thermostatting and rigid zones at its boundaries.

oriented with (100), (110) and (111) surfaces; each surface is scratched in 2 different directions. The orientation of the scratching directions, the extensions and the number of atoms used in the Fe substrates are assembled in Table 1.

In order to prevent any center-of-mass motion of the substrate during the simulation, we fix two atom layers of the substrate at the bottom of the simulation cell [28]. The next four layers at the bottom as well as the outermost four layers of the substrate in lateral directions are kept at 0 K by a velocity-scaling thermostat. We note that we performed additional simulations at 300 K for the (100)[011] scratch system in order to assess the temperature dependence of our simulation procedure; the results are discussed in Appendix B. The top surface is free. Further details of the simulation method have been reported elsewhere [30].

The Mendelev potential [34] is employed to describe the Fe–Fe interaction in the substrate; we note that this potential has a cut-off radius of 5.4 Å. A purely repulsive potential is used to model the interaction between the C atoms of the diamond indenter and the Fe atoms of the substrate; this potential is obtained from a Lennard-Jones potential describing the C–Fe interaction [35], by cutting it off at 4.2 Å at its minimum and then shifting it such as to have continuous energy and force at the cut-off radius.

The Fe substrate is relaxed before starting the simulation until all stress components have reached values $< 10^{-5}$ GPa, as recommended previously [12]. Then the center of the indenter is positioned at a height of 26 Å above the substrate surface; there C and Fe atoms do not interact. The indenter velocity is set to $v = 10$ m/s, both in the indentation and in the scratching process. The so-called velocity-controlled mode is used for performing the simulation; that is, at every MD time step Δt, the indenter proceeds rigidly by a path length $v \cdot \Delta t$. We study scratching depths d equal

Table 1
The axis orientations used in the 6 scratching simulations, the respective dimensions of the substrate, and the number of atoms N in the substrate. z denotes the normal direction of the substrate surface, and x the scratching direction along the surface.

Substrate	x, y, z	Dimensions (Å)	N
1	[010], [001], [100]	314 × 228 × 200	1,240,800
2	[011], [0$\bar{1}$1], [100]	323 × 202 × 200	1,128,000
3	[$\bar{1}$10], [001], [110]	485 × 428 × 202	3,636,000
4	[001], [1$\bar{1}$0], [110]	428 × 485 × 202	3,636,000
5	[1$\bar{1}$0], [11$\bar{2}$], [111]	323 × 233 × 247	1,602,134
6	[11$\bar{2}$], [$\bar{1}$10], [111]	326 × 242 × 247	1,683,226