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A quantitative and comparative study of sputtering yields in Au

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Abstract

We have systematically tested two entirely independent, empirical potentials (EAM and MD/MC CEM) which are widely used in classical molecular dynamics simulations by simulating Xe ion impacts to the Au(1 1 1) surface in the broad energy range between 0.1 and 200 keV. Special attention is paid to ensure that the simulated results are statistically significant. We have also compared simulations to experimental results on sputtering yields and crater production. Both potentials bring about qualitatively similar outcomes of the collision cascades, giving good confidence that the previous conclusions drawn from simulations on heat spike behaviour in dense metals are valid. However, the quantitative results are different. The MD/MC CEM potential has clearly better agreement with experimental sputtering yield data than the EAM potential, although neither potential agrees with experiments in the full energy range studied.

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1. Introduction

Heavy ion bombardment of heavy metals at kiloelectron volt energies is a prototype of ion irradiations where heat spikes are important for the outcome of collision cascades. The topic has been studied much by both experiments and computer simulations, giving a good qualitative picture of what happens. However, few studies have attempted to test whether it is possible to obtain quantitative agreement between theory and experiment, which would give good confidence that the qualitative conclusions drawn from simulations are reliable.

Brinkman proposed in 1954 that an energetic ion in a dense material may not only displace a

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few isolated atoms, but in fact for a brief time produces entirely empty regions surrounded by a highly overdense one [1]. Ever since then the precise nature and even the existence of such heat spikes, also called collisional spikes or thermal spikes, has been subject to debate. The very high temperature (thousands of kelvins) and short time scale (a few picoseconds) associated with the heat spikes make them an entirely non-equilibrium phenomenon. Hence it was not clear for a long time whether ordinary thermodynamic concepts can be used at all in describing the spikes. Also the most common tool to simulate irradiation effects, the binary collision approximation [2], is not suitable to simulate heat spikes since it breaks down when the recoil energies approach thermal energies. It was only in the 1980s when computer capacity advances made it possible to simulate collision cascades using molecular dynamics [3–5] that a certainty of the nature of heat spikes started to emerge. By now it is clear that heat spikes do exist and in fact resemble surprisingly much the original prediction of Brinkman [1].

Two of the main evidences of heat spikes are related to surface effects of ion irradiation. Sputtering yields have been observed to increase nonlinearly with energy when heavy ions bombard heavy metals [6–10]. Also the surface morphology changes due to irradiation, especially the formation of craters and even more exotic structures [11–14], is hard to explain with any other mechanism than the liquid flow from heat spikes [15,16].

Molecular dynamics (MD) simulations have been invaluable in giving understanding of sputtering and crater formation from heat spikes [17,15,16,18–22]. Most of the studies to date have, understandably, focussed on obtaining qualitative understanding of the atom displacement mechanisms, employed a single atomic interaction model, and considered only a few ion energies. It would, however, be very useful to know how reliable the models are quantitatively, and whether agreement with experiments in a narrow energy range implies that the model used is reliable in a wider one. The cluster emission study by Colla et al. [18] is an example of quantitative comparison of simulations to experimental results.

In this work we address these questions by simulating Xe ion impacts on Au(1 1 1) surfaces at ion energies varying from 0.1 to 200 keV, i.e. more than 3 orders of magnitude. We chose this particular system because there is good experimental data available on both the sputtering yield [23] and crater formation [13,14]. We also simulate Ar impacts at energies 1–5 keV, another case where good experimental data on sputtering from a single-crystalline Au(1 1 1) surface is available. We employ two different interatomic potentials, the EAM [24] and MD/MC CEM [25] ones. Both are conceptually based on the effective medium theory but are otherwise very different in the approach to their derivation. Hence comparing results obtained with the two potentials provides a good test base on how sensitive the qualitative and quantitative sputtering yield results are to the potential choice. In addition to the EAM and CEM models used in this work, there are numerous other many-body potential schemes for metals (see e.g. [26,27,29,30,80] and references therein).

We pay special attention to get statistically reliable values for simulated sputtering yields and other quantities. The experimental sputtering yield is an average of numerous sputtering events. To be able to compare experimental and simulated yields, the series of simulation runs should be long enough to prevent an individual run to change considerably average yield or other physically interesting values. Especially at high energies, the yield can vary from zero to several thousand atoms per ion between individual simulated events. If the simulation series is too short, the average yield can for instance double after adding a single new event in the series.

2. Methods

2.1. Overview of potentials

The interatomic potentials based on the effective medium theory (EMT) are and will be a very important practical tool for large scale MD simulations, and thus the knowledge of their proper application areas are of great importance. In spite of the drawbacks, the potentials provide very