

A Molecular Dynamics Computer Simulation Study  
of the Damage Produced in Metal Target  
Surfaces During Ion Bombardment

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## 1. Introduction

Molecular dynamics simulations now study the damage created in metal surfaces by bombarding ions [1-5]. The computer model used in atom ejection studies [6] has been extended to cool and recrystallise the target. The target's response is physically plausible, and its final configuration is consistent with transmission electron microscope (TEM) studies of ion-bombarded target surfaces. Here the chief emphasis will be placed on effects which will influence the outcome of a SIMS experiment.

## 2. Preliminaries and the Model

The results reported here are little influenced by the type of potential function used to describe the ion-atom interaction. All effects discussed below are observed with several potential functions. The ion-target system is  $\text{Cu}/\text{Ar}^+$ ,  $\text{Cu}/\text{O}^+$  or  $\text{Cu}/\text{U}_2^+$ . Cu is a face-centered cubic (fcc) material.

The model examines the first 8-10 layers of target material, approximately 2000 atoms. After an atom ejection trajectory the modified program cools the resultant molten target (mean energy/atom is of the order of 2.0 eV). Energy is withdrawn by a total energy dependent frictional mechanism, like thermal conduction [2]. If the mean energy/atom deposited in the target volume is not large, recrystallization nucleates on undamaged portions of the target. The program starts recrystallization of heavily damaged targets at the boundaries. This artificial method produces final results similar to those found in less damaged targets [2].

The atoms/single ion (ASI) distribution of a simulation [6] is a fundamental attribute of the atom ejection process which is not, as yet, accessible to experimental study. In the simulations some ions eject many atoms, and often, some eject none. For certain types of systems a zero ASI is most probable. The large probability of low ASI values guarantees that some large ASI trajectories exist in every experimental system, and that high ASI trajectories produce a major fraction of all ejected atoms.

This paper deals with high damage trajectories. Although their number is small, never more than 5-10 percent of the total number of ions, they dominate all observable effects in all atom ejection experiments, including SIMS. They differ strikingly from trajectories which produce average ASI values.

At ion energies above 20 keV, the TEM indicates that pits form in metal targets [7-9]. These pits have been interpreted as evidence for spike effects, high energy-density cascades, and the breakdown of linear cascade theory [10,11]. Recent simulations indicate that high energy-density cascades can occur at low ion energies [1]. Large ASI value trajectories create major surface damage and are responsible for pit formation [1]. Pit formation correlates with a high ASI value because both are produced similarly, but many atoms from the pit are not ejected from the surface.

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**SJ Ball**



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