SURFACE EROSION AND MODIFICATION BY ENERGETIC IONS

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Interactions of Gas Cluster Ion Beams (GCIB) and Highly-Charged Ions (HCI) with solid surfaces have fundamental and practical interests in such areas as nuclear fuels [1], TeV accelerators [2], and extreme ultra-violet lithography (EUVL) source devices [3], HCI driven SIMS for surface analysis [4], protein desorption by HCI impacts [5].

Mitigation of high voltage rf breakdowns and Q-slope is a major concern in development of higher-field RF cavities for next generation accelerators [3].

Surface treatment by GCIB method has recently been proposed as a new way to significantly reduce the surface roughness and the dark current from the rf-cavity surfaces and enabling operation at higher acceleration gradients [6].

SIMULATION MODELS

As an HCI ion approaches a metal or semiconductor surface, the strong Coulomb field of HCI can pull the electrons from the solid surface into the Rydberg states of the ion [7]. The hollow atom (HA) is formed which evolves further by emitting electrons and/or photons via the Auger processes. The potential energy of Xe^{+q} ($q \leq 54$) is calculated by a multi-configuration Dirac–Fock method [8]. The classical over-the-barrier (COB) model [7, 9] is widely used to estimate the distance where the first resonant charge transfer can take place. The life time of HA is much greater than the interaction time: $\tau_I \sim 10^{-13}$ s [10]. Another physical effect that should be taken into account is electric field screening. We used the screening length for the Coulomb forces between the ions to be 5Å which is of the order of the Si lattice parameter. A detailed analysis of the previous work on screening processes has been given in Ref. [11, 12]. An excessive charge inserted into plasma with will be neutralized within a characteristic time called the Maxwell relaxation time. This time could be obtained by a solution of the static Maxwell equations: $N_q(t) = N(0)\exp(-t/\tau)$, where $\tau = \varepsilon\varepsilon_0/\sigma$. Here, N_q *(t)* is the total number of charges at a time *t*. ε and ε_0 – are the electrical permittivity of a material and vacuum, respectively. The above formula for N_q was first proposed by Bringa and Johnson in [11, 12], without referring it to the Maxwell relaxation time. MD models were developed for various materials that included Si, Al, Cu, Ni, W, and Nb. The Stillinger-Weber and Born-Mayer potential functions were used for Si [13, 14], and a Finnis-Sinclair potentials for bcc tungsten and niobium [15].

The sputtering yields as a function of the potential energy of Xe^{q+} were studied.

The mesoscale surface dynamics equation represents the nonlinear dynamics of growing surface profiles in terms of the coarse-grained interface heights $h(\boldsymbol{r},t)$ in a d-dimensional space where $\boldsymbol{r}$ is the radius-vector in a (d-1)-dimensional plane at time t, and accurately describes behavior in later-stages, or scaling properties, of a growing interface and can be found elsewhere [6].

SIMULATION RESULTS

The calculated and experimental results [8] for the sputtering yield shown in Fig. 1 were obtained for a highly-charged Xe^{+q} ion, with a kinetic energy of 1 KeV, bombarding a Si (100) and a W (100) surfaces. Although the recently developed microbalance technique [17] allows one to measure the frequency shift and calibrate the experimental device against the absolute surface erosion characteristics, there are still no available experimental data for the sputtering yields of Si surfaces induced by Xe^{+q} HCIs. The calculated data were also compared to the experimental sputtering yields obtained for LiF, SiO_2, and GaAs in [8, 18].

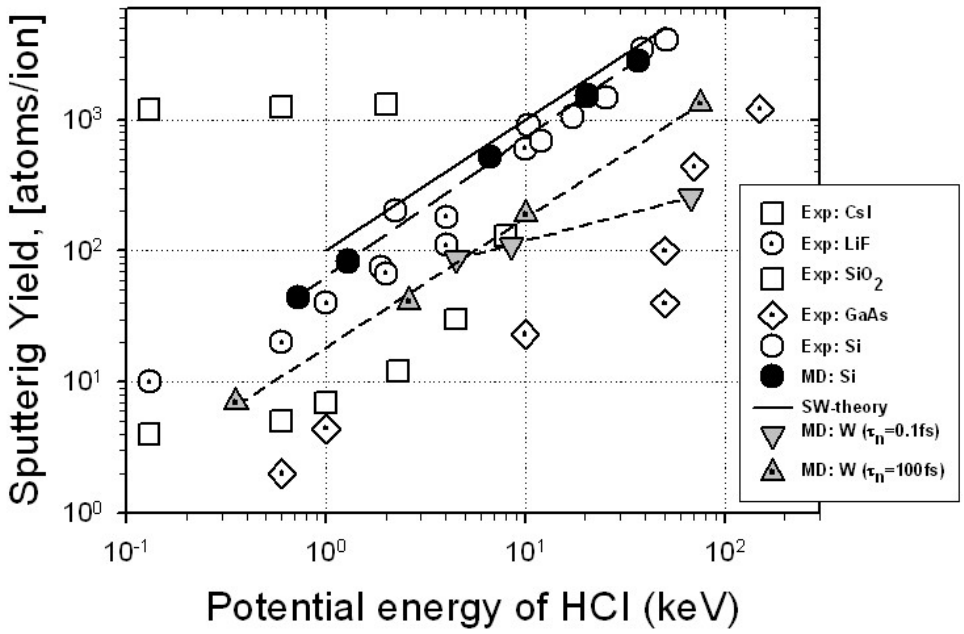

Fig. 1. Comparison of calculated sputtering yield for Si and W surfaces with experimental data available for various materials: CsI, LiF, SiO2, GaAs [8, 18]. The dashes are linear fits to the data points and MD data. The tungsten yields are calculated for two neutralization times: τ_n = 0.1 and 100 fs. The solid line is drawn according to a simple shock-wave theory model [19].

There are clearly seen two characteristic energy intervals where the sputtering yields have a linear power-law dependence (above 0.1 keV for Si), and a constant (below that threshold

value). The threshold energies for these two energy regions are almost the same for CsI, SiO2, LiF, and Si. However, the threshold is much bigger for GaAs. One reason for such behavior could be a very low intrinsic density ($n_i = 2\times10^6$ cm^{-3}) of the carriers in GaAs at room temperature. The solid line in Fig. 1 is drawn according to a simple shock-wave theory model [19] which predicts a linear dependence of the sputtering yield on the total Coulomb energy. The tungsten sputtering yields were calculated for various neutralization times τ_n =0.1, 1, 15, and 100 fs. Shock wave generation was studied for a Xe^{+44} HCI impact on a Si (100) surface.

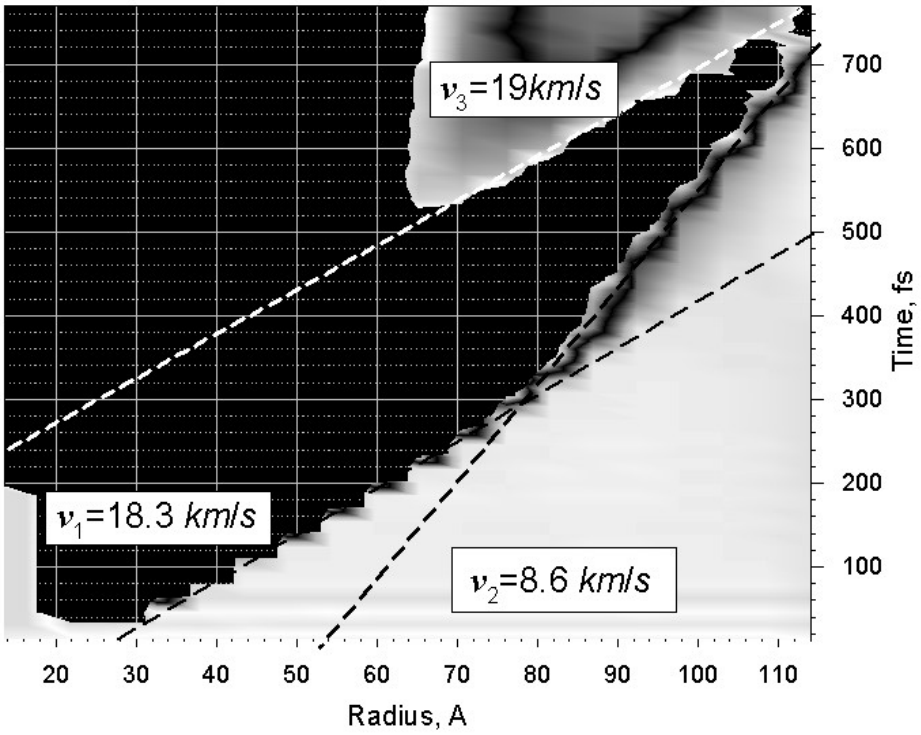

Fig. 2. The radial kinetic energy of the target atoms on time and radial distance from the collision spot on the top of the Si target .

Fig. 2 shows the dependence of the radial kinetic energy on time and radial distance from the collision spot on the top of the Si target. These figures reveal two different shock waves, with the velocities of 18.3 and 19 km/s for the forward and rarefaction waves, respectively. After a few hundreds of fs, the forward wave decays and propagates with a slow wave velocity, of 8.6 km/s, which we should relate to a longitudinal acoustic wave.

Velocity distribution of the ejected atoms reveals the mechanism of sputtering – the shock wave mechanism gives a v^{-3} dependence at higher velocities which can be obtained from the shock wave theory [16, 19].

Fig. 3 shows a crater shape obtained by our MD simulations. It shows the crater formed by an accelerated Ar_{429} cluster with the kinetic energy of 125 eV/atom.

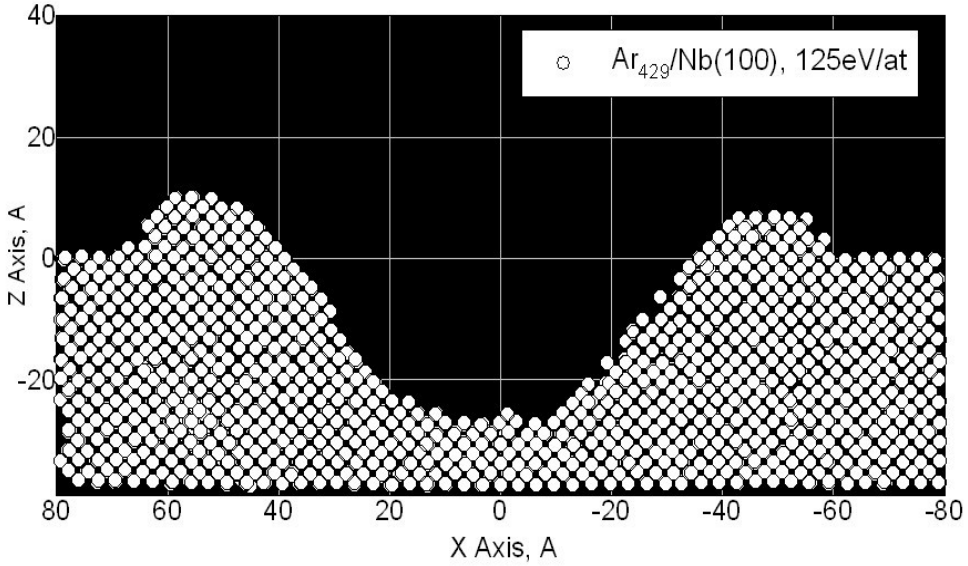

Figure 3. Crater shape obtained by our molecular dynamics simulations formed by an Ar_{429} cluster impact with the kinetic energy of 125 eV/atom.

A preliminary analysis based on the local atomic stresses and on the slip vector calculation showed that both the GCIB and HCI craters strongly emit dislocation loops and stacking faults that are located near the surface and are stable for the whole period of simulation which was 75 ps. The maximum calculated shear stress for the tungsten target was well above the lattice strength and the tungsten bulk modulus. Such extended defects can easily be the driving force for the surface hillocks observed on the top of conductive surface irradiated by HCI and by high-energy heavy ions.

We modeled surface modification of a Nb surface containing two types of surface tips, with greatly different sizes: one of the tips was a narrow and tall hill, with the diameter of a few nm, and the second tip was modeled with a wide and short hill having a typical area of a many tens of nm. The results of the first high voltage test of a GCIB treated electrode will be discussed [20][1]. Recent measurements have shown a "dramatic reduction" in the number of field emitters of Nb SRF cavity material.

Experimental data on *Q*-slope iclude a number of mechanisms. These include: 1) Magnetic field enhancements due to surface irregularities, 2) interface tunnel exchange, where the electrons are affected by the presence of states in the surface, 3) thermal feedback, magnetic field dependence of the energy gap, 4) grain boundary effects, and a variety of other models.

[1] These experimental results were provided by C. Sinclair and his group at Cornell University.

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