COMPUTER SIMULATION OF SURFACE MODIFICATION WITH ION BEAMS*

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Abstract

Niobium surface modification dynamics treated by cluster ion irradiation was studied based on atomistic and mesoscopic simulation methods and the results were compared to experiments. A surface smoothening method was proposed consisting of a treatment of the Nb cavity surfaces by accelerated gas (argon) cluster ion beams (GCIB) that is capable of reducing the surface roughness up to the theoretical limit.

INTRODUCTION

Higher voltage gradients are required for development of future TeV linear accelerators and muon-muon colliders. However, the development of these accelerators and colliders is seriously hampered by electrical breakdown in the vacuum between the electrodes in the accelerator structures, power sources, and waveguides. Electrical breakdown in vacuum, for both *rf* and *dc* systems, has been studied for many years, and many mechanisms have been proposed to explain this phenomenon [1-4]. The *rf*-vacuum breakdown occurs in either copper ("warm") or niobium superconducting ("cold") cavities and one of the possible mechanisms at high electric field gradients as 10 GV/m is due to electrode surface irregularities including scratches, whiskers, crater rims, cracks, grain boundaries, oxidized areas, organic absorbed species, and dust particles.

Breakdown seems to have a sharp threshold in electric field, but somewhat weak dependence on frequency, temperature of structure, and vacuum conditions [5, 6]. Recent experiments have shown that breakdown occurs when the tensile stress exerted by local electric fields becomes comparable to the tensile strength of the metal [6]. While single atoms may not interact strongly with the electric fields, the emission of clusters and fragments, in the presence of field emitted electron beams, may produce very high local power densities (10^{13}-10^{14} W/cm^3), which could rapidly ionize and damage the structure [7]. Field emitted electrons could easily ionize such atomic clouds at the near-surface region and form plasma that may erode the cavity surface.

Although the surface electric field gradients are relatively small for the superconducting Nb cavities, a new development of multilayer coatings shows that the the critical magnetic fields can be significantly increased, thus enabling much higher acceleration gradients, comparable to those of "warm" cavities [8]. In this case, the high-voltage surface rf-breakdown will still be a limiting factor for the Nb-cavities. Nanoscale surface features are also widely believed to play an important role in other breakdown mechanisms of SRF cavities such as local quenching [9]. These will be addressed in future papers, but our present work already shows that there are excellent prospects that GCIB surface treatments may also be effective for reducing these as well.

This paper describes the results of our further development of the cluster field evaporation model, recent atomistic and mesoscopic simulations of a Nb surface modification by cluster ion beams.

FIELD EVAPORATION MODEL DEVELOPMENT

In our previous work [10] we showed that a new physical effect exists that consists of tearing out a small chunk (cluster of atoms) of the surface material in a high surface electric gradient and such metal clusters will fill out the near-the-surface region of the cavity. They could easily be ionized by the dark-current and hence hit back the cavity surface leading to the vacuum breakdown. Based on the analysis of the available experimental data and existing theoretical models, a new concept of plasma formation and surface breakdown model was developed. An atomistic simulation model of the vacuum high-voltage breakdown is developed and applied to a study of a picosecond-scale dynamics of the nanometer scale tip on the top of the cavity surface under applied high-voltage gradient.

Experiment on the vacuum breakdown in *rf*-field shows that the critical breakdown field is almost independent of the cavity temperature [5]. Our results also predict a rather weak temperature dependence of the critical field. There is no experimental work done in finding cluster evaporation in *rf*-field. However, this phenomenon is well studied for *dc*-electric fields. The *dc*-field experiments show a failure of the tip because an image cannot be obtained by such a tip; and therefore, it is an undesirable event.

Our work predicts that single ions have higher critical fields compared to those of a group of atoms, which makes cluster ions to be more susceptible to field-evaporation in a high-gradient *rf*-field. However, this does not mean that single ions will not be evaporated in a high-gradient *dc*-electric field. The geometry of the tips is changing continuously during the experiment and at different time instants surface can emit groups or single ions, depending on the local tip's geometry.

Coulomb explosion of the field-evaporated highly-charged cluster ions, interaction of such clusters with the rest of the surface, heating of clusters by dark-current

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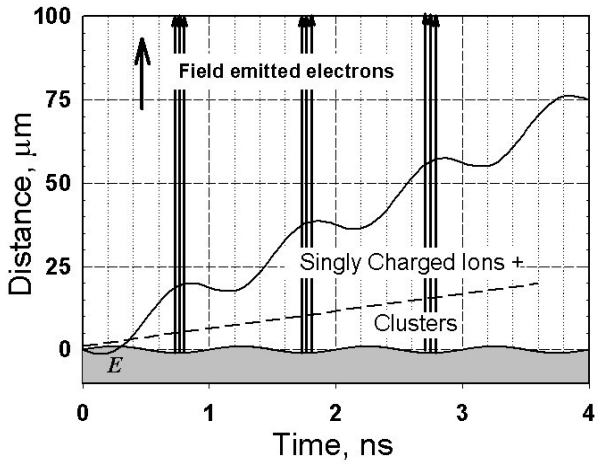
electron emission would significantly contribute to the understanding of the vacuum breakdown triggering mechanism. They will be the subjects of further improvement of the new concept.

There is a need for specific experiments to detect, observe, and study such clusters to verify the new mechanism of vacuum breakdown studied in this paper.

Figure 1 shows behavior of ions emitted from asperities in an electric field of 50 MV/m [7]. The initial ion velocity comes from the local field of 10 GV/m operating over dimensions of 0.1 μm. Field emitted electron beams are produced when the electric field reverses, and these electron beams can further ionize the ions near the emitter.



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SURFACE DYNAMICS SIMULATION

Atomistic simulation

In the present work, we study the surface smoothening processes triggered by irradiation of the surface with cluster ions Ar_n (n = 92) having various kinetic energies of 12, 27, and 54 eV/stom on a rough Cu surface. The details of our Molecular Dynamics simulation method could be obtained elsewhere [11].

From 1 to 10 pyramidal hills, with the heights of about 5-15 nm, were placed on the top of a Cu (100) surface and the simulation was followed up to 50 cluster impacts. The total simulation time was of about 600 ps.

Fig. 2 shows the dose dependence of the surface average heights (the residual surface roughness) of a rough Cu surface irradiated with multiple cluster collisions calculated in this work. As this figure shows, the roughness decreases rapidly at of about 50eV/atom, which is in the energy range where the lateral sputtering phenomenon occurs [11]. Below this energy, the surface becomes more rough.

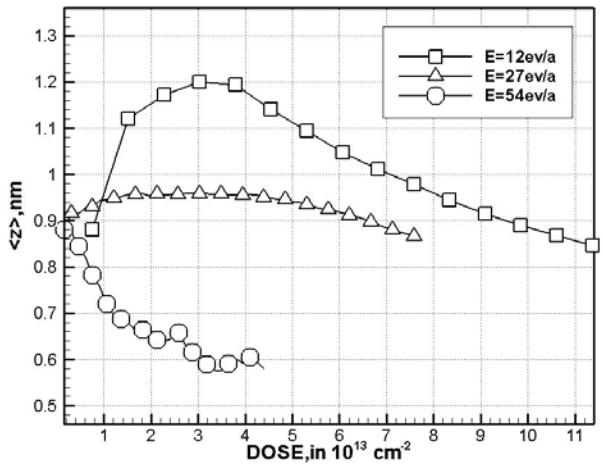

Figure 2. Dose dependence of a Cu surface heights irradiated with multiple Ar_n clusters at three different energies calculated by Molecular Dynamics. Low energy beams can make surface more rough. Smoothening occurs at the energies near and above 54 eV/atom.

Figure 3 shows the experimental dose dependence of the surface average heights and the standard deviation R_a of a Cu surface [12]. The experimental cluster energy was 30 KeV and the cluster size had a broad maximum at of about 3000 atoms in a cluster.

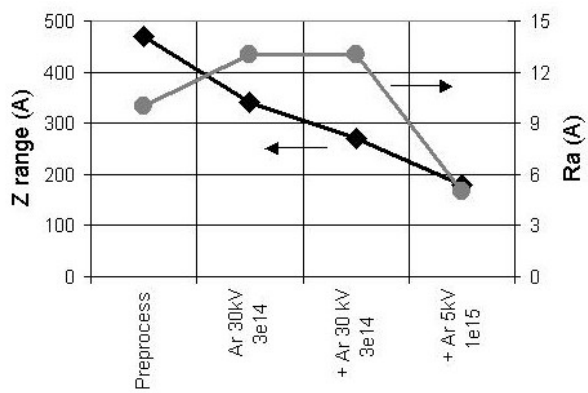

Figure 3. Experimental results for the roughness (standard deviation - R_a) and average heights (<z>= Maximum - Minimum height) dependence on the ion dose of an isolated asperity on a smooth Cu surface bombarded with Ar_n cluster ion beams. The processing occurred in three steps as noted on the figure. After each irradiation process step the sample was removed and measured using AFM. Fiducial marks were used to relocate the same asperity after each step. The irradiation doses $+3\times10^{14}$ and $+1\times10^{15}$ on the x-axis mean the total dose of 3×10^{14} at 30 kV and 1×10^{15} ions/cm^2 at 5 kV additionally to previous dose of 3×10^{14}, respectively.

A direct comparison of these two results is difficult due to the difference in the cluster size. However, our simulation qualitatively reflects the trend which is shown in the experiment: starting from certain cluster ion energy,

the surface roughness decreases and reaches a level defined by a maximum ion dose.

Mesoscale simulation

The dynamics of a non-equilibrium surface profile could be determined from continuum surface dynamics equation:

$$\dot{h}(r,t) = \mu\nabla h(r,t) + \nu\Delta h(r,t) - k\nabla^4 h(r,t) + f_{cr}$$

Where, $\mu=\gamma/\eta$, γ is the surface tension, η is the viscosity, ν is the term which accounts for the evaporation and deposition processes, κ is the coefficient which is related to the surface diffusion coefficient, $f_{cr}(\nabla h)$ is the crater formation term, which depends on the local surface slope. This equation represents the nonlinear dynamics of growing surface profiles in terms of the coarse-grained interface heights $h(\mathbf{r}, t)$ in a 3-dimensional space where $\mathbf{r}$ is the radius-vector in a 2-dimensional plane at time t, and accurately describes behavior in later-stages, or scaling properties, of a growing interface. The nonlinear term conserves the surface current, and a white noise term is not shown.

The typical irradiation parameters used for surface smoothing are as follows: cluster ion doses are in the range of 10^{12} - 10^{15} ion/cm^2, average cluster sizes are in the order of 10^2-10^5 atoms, the total cluster energies is 30 keV. A single hill, having a typical area of order 10^6 - 10^7 Å^2, was placed in the center of the computational cell. The model cluster dose was in the order of 10^3 - 10^4 cluster/hill. Clusters hit the surface normally at a random position. Displacements of surface particles after the cluster impact were modeled in accordance with a probability, obtained in our MD simulation of single cluster ion impact on a flat surface.

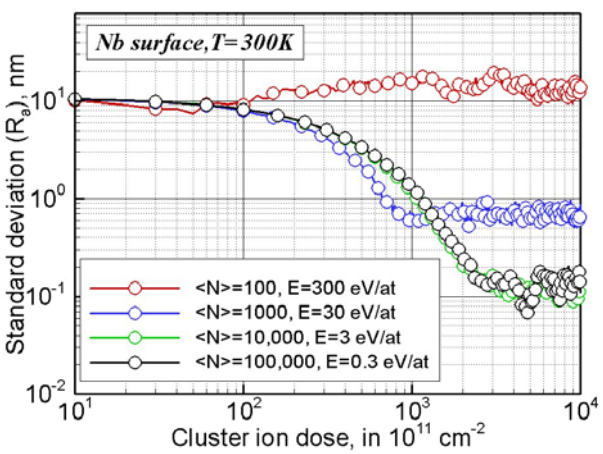

Figure 4. Dose dependence of the average surface roughness (R_a) for cluster ion beam treatment of a Nb surface, with the total cluster energies of 30 KeV and average cluster sizes of 100, 1000, 10,000, and 100,000, obtained by this mesoscale simulation. The energies per atom are given in the inset.

Fig. 4 demonstrates the results of our mesoscale simulations for the Nb surface smoothening. Four different cluster sizes were modeled, where the total energy of the cluster ion was kept at 30 KeV that is typical for experiments with cluster ions. For the ion energies per atom higher than 30 eV, the roughness tends to saturate at some irradiation dose. The residual roughness is always defined by the geometry of an individual crater and it increases with the increase of the total cluster ion energy.

The simulation predicts that the lower energies per atom (at the same total energy) produce much smoother surfaces which correlates well with the experimental results shown in Fig. 3.

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