MS381

ADVANCED SURFACE POLISHING USING GAS CLUSTER ION BEAMS

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Abstract

The gas cluster ion beam (GCIB) treatment can be an important treatment for mitigation of the Q-slope in superconducting cavities. The existing surface smoothening methods were analyzed and a new surface polishing method was proposed based on employing extra-large gas cluster ions (X-GCIB)

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1. INTRODUCTION

Higher voltage gradients are required for development of future TeV linear accelerators and muon-muon colliders. However, rf high-electrical gradient breakdown in the vacuum between the electrodes drastically reduces the critical electric field which such structures can sustain [1]. Various breakdown mechanisms were analyzed and a new cluster field evaporation mechanism was proposed in our previous papers [2-6].

When the electric field increases to 25-30 MV/m, a significant decrease of the quality factor Q_0 has been observed by many groups (CEA, JLab, DESY, KEK) [7]. This phenomenon that degrades the superconducting cavity properties is called high-field Q-slope. The study and treatment of the Q-slope is a very important problem for the future ILC deployment.

This paper describes a recent development of the rf-breakdown and thermal quenching mitigation. We present the results of atomistic simulations of an Nb (100) surface irradiated with argon and oxygen cluster ions and show recent Nb surface smoothening results.

2. FIELD EVAPORATION MODEL DEVELOPMENT

In our previous work [2] 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.

Figure 1 shows behavior of ions emitted from asperities in an electric field of 50 MV/m [3]. 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. To mitigate this phenomenon, the cavity surface should be smoothed to an angstrom level.

Analysis of the surface preparation/smoothing methods shows that the buffered chemical polishing, used for the surface preparation of the linear collider rf-cavity surfaces is not satisfactory. The Electrolytic Polishing method has recently been developed as a new rf-cavity surface preparation method and it is used in surface treatments of the x-ray telescope mirrors for astrophysics, where it is called super-polishing. Figure 2 shows comparison of the existing surface smoothing methods with the GCIB method [8-12]. We have also provided a future development of the gas cluster technique based on using eXtra-large gas clusters, which we called X-GCIB [4]. Our theoretical estimates and atomistic simulation predict that this new development of the method could provide a theoretical limit for the ultimate surface smoothening.

3. Q-SLOPE MITIGATION BY GCIB TREATMENT

Nanoscale surface features are also widely believed to play an important role in other breakdown mechanisms of SRF cavities such as local quenching or Q-slope [13]. Achieving the acceleration voltage of 35 MV/m in the main linac superconducting cavity is an important goal for the future International Linear Collider (ILC). Although a treatment for Q-slope exists, consisting of a modest temperature annealing (baking), the understanding of its causes is still lacking.

One explanation of the baking effect is that the high purity bulk Nb may be covered by a thin (~2 nm) layer of "low-grade" Nb with a lower critical magnetic field, which dissolves into the bulk after baking. The impurity interstitial oxygen, strongly depresses superconductivity in Nb at several atomic %. Baking increases the grain-boundary de-pairing current density (to be shown yet experimentally). The effect of grain-boundaries (GB) on the RF surface resistance is important and GBs are the weak links. The most important input parameter is the GB critical current density together with the grain size. Various existing models for the Q-drop and baking effect are summarized in Table 1 [7, 14-16].

A broad theoretical and experimental program is needed to study Nb oxide formation and structure at the first 100 nm of the surface and at the grain boundaries, formation and diffusion of interstitial defects, decomposition of thermal oxide layers, defect clustering and decomposition, and finally the feasibility of Nb carbide formation which may affect the Q-slope. These will be addressed in future work, but our present work already shows that there are excellent prospects that GCIB surface treatments may also be effective for reducing these as well.

4. CRATER FORMATION ON A NIOBIUM SURFACE

In the present work, we studied the surface smoothening processes triggered by irradiation of the surface with atomic Ar_n and molecular clusters $(O_2)_n$ (n = 400-1000) having various kinetic energies of 50-125 eV/atom on a flat and rough Nb surfaces. The details of our Molecular Dynamics simulation method can be obtained elsewhere [17]. The rectangular surface slab containing up to 400,000 Nb atoms interacting via an improved Finnis-Sinclair potential [18,19] was brought into equilibrium at room temperature and bombarded by argon atomic and oxygen molecular clusters. To treat the chemically reactive oxygen bombardment of the Nb surface, a simple chemisorption model was developed that takes into account a large chemical reaction energy (~ a few eV per oxygen molecule) to be released during the close proximity of the oxygen molecules to the Nb surface.

Fig. 3 shows two crater shapes that were obtained by our molecular dynamics simulations. Fig. 3 a) shows the crater formed by an accelerated Ar_{429} cluster with the kinetic energy of 125 eV/atom. Fig. 3 b) shows a much shallower crater formed by an $(O_2)_{429}$ cluster with an energy of 50 eV/molecule (or 100 eV/atom). As a result of the oxygen cluster collision, the craters are shallower than those created by gas clusters that are chemically inactive. We found that the reflected oxygen and the ejected niobium particles show more salient lateral features than that of an inert gas cluster impact. Our preliminary studies showed that the oxygen cluster impact is capable of providing a larger lateral sputtering effect than that of the chemically inactive argon beams. As a result, we expect that oxygen cluster beams will demonstrate much higher surface smoothening effect compared to a non-reacting gases.

5. MESOSCALE SIMULATION

The dynamics of a non-equilibrium surface profile could be determined from continuum surface dynamics equation [21]. 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 10^3 atoms or molecules, and the total cluster energies is 30 keV.

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. These two types of the tips are shown in Fig. 4. The total modeled area was in the order of 10^6 - 10^7 Å^2, and this area was irradiated by up to 1000 large oxygen 30 keV clusters. The clusters randomly bombarded the whole area of the simulation cell. The cluster dose was in the order of 10^3 - 10^4 cluster/cell. Displacements of surface particles after the cluster impact were modeled in accordance with the probability, obtained in our MD simulation of a single cluster ion impact on a flat or inclined Nb surface.

Fig. 4 demonstrates the results of our mesoscale simulations for the Nb surface smoothening. 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 showed that the narrower hill is removed by an irradiation dose that five times lower than the blunt hill. The larger the surface bump is in the horizontal plane, the higher irradiation dose is needed to completely remove the hill and smooth the surface. It is known that the narrower hills have a higher chemical potential than those with a larger diameter. Therefore the surface treatment by chemically inactive GCIB should remove narrow hills faster than the bigger ones. The effect of the oxidation on various hills and its predominant selectivity of various hill sizes is unknown.

We expect that the surface roughness will mostly be defined by the physical removal of the hills rather than that by the chemical reaction.. Similar results were obtained in Ref. [22] where crater shapes on HOPG were determined for different angles of incidence and the motion of the ejected materials was evaluated by a Monte-Carlo model to show the effect of processing. The authors [22] concluded that narrow ripples smoothed much faster than broad ripples even when you started with the same Ra (i.e. the same amount of material to be flattened).

Figure 6 shows the recently published results of the first high voltage test of a GCIB treated electrode [5]. The field emission of a 150-mm diameter stainless steel electrode was measured as a function of the gap field. This electrode was treated using a sequence of high and then low energy Ar, for smoothing followed by high and then low energy O_2 to improve the oxide characteristics. Figure 6 shows a comparison of this electrode to a typical non-processed electrode. In spite of the fact that the initial mechanical polish was inferior on the GCIB processed electrode, the processing caused a reduction of 6 orders of magnitude of the field emission. At this point the relative contributions of the surface smoothing and the thicker, harder oxide to this very encouraging result cannot be determined.

5. SUMMARY

The existing surface smoothening methods were analyzed and compared and a new surface polishing method was proposed based on employing extra-large gas cluster ions (X-GCIB). Q-slope models were discussed and a new mitigation method was proposed. Niobium surface treatment by cluster ion irradiation was studied based on atomistic and mesoscopic simulation methods and the surface modification dynamics results were compared to experiments.

Acknowledgments

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Figure Captions:

Figure 1: Behavior of ions emitted from asperities in an electric field of 50 MV/m. The initial ion velocity is due to the local field of 10 GV/m operating over dimensions of 0.1 m. Field emitted electron beams are produced when the electric field reverses, and these electron beams can further ionize the ions near the emitter.

Figure 2. Surface roughness obtained with various surface polishing techniques. *The following abbreviations are used:* CMP – Chemical Mechanical Polishing [1,2], MRF – Magneto-Rheological Polishing, TCP – Tribochemical Polishing, SP – Superpolishing for astrophysical mirrors, GCIB – Gas Cluster Ion Beam surface smoothing technique, XL-GCIB – future extra-large GCIB technique that is our goal. SP is a technique that combines metal electroplating with magnetron sputtering deposition, i.e. it is not a true smoothening process but rather a multi-stage process that includes various methods.

Figure 3. Crated formed with a) a single Ar_{429} at 125 eV/atom and b) oxygen molecular clusters $(O2)_{429}$ E=100 eV/atom, calculated by Molecular Dynamics.

Figure 4. The results of the mesoscale modeling of the Nb surface modification irradiated by oxygen molecular cluster ion beam at a dose 10^{13} ions/cm2. The cluster energy was 30 KeV and

the cluster size was of about 3000 oxygen molecules in a cluster. The surface contained two types of tips: narrow and tall and wide and short.

Figure 5. Field emission measurement for unprocessed (squares) and GCIB processed (circles) stainless steel electrode material (reprinted from reference [5]).

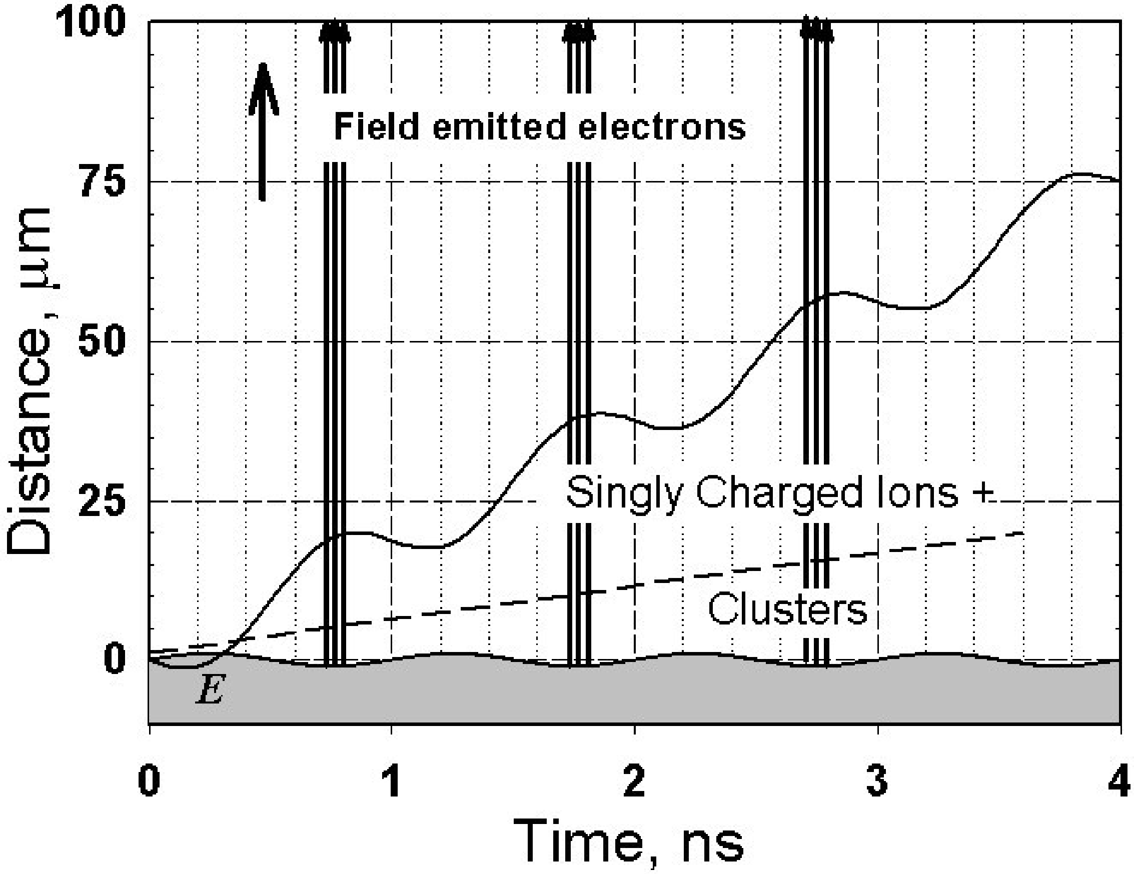

100
75
50
25
0
Distance, μm
Field emitted electrons
Singly Charged Ions +
Clusters
E
0
1
2
3
4
Time, ns

Figure 1

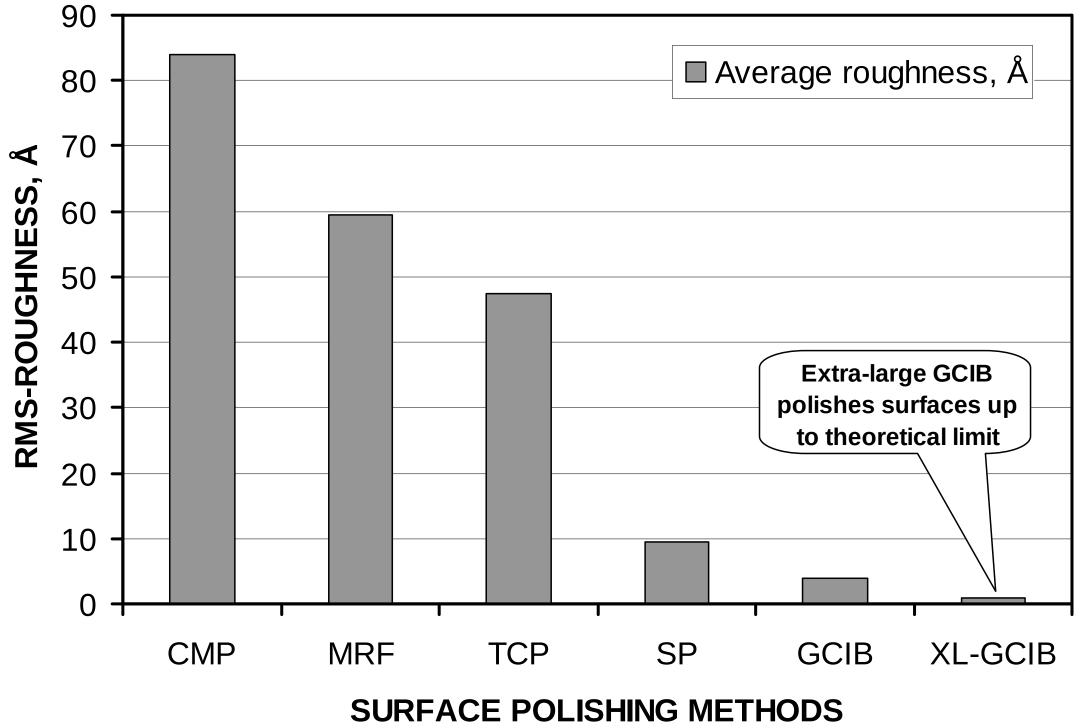

90
80
70
60
50
40
30
20
10
0
RMS-ROUGHNESS, Å
Average roughness, Å
Extra-large GCIB polishes surfaces up to theoretical limit
CMP
MRF
TCP
SP
GCIB
XL-GCIB
SURFACE POLISHING METHODS

Figure 2

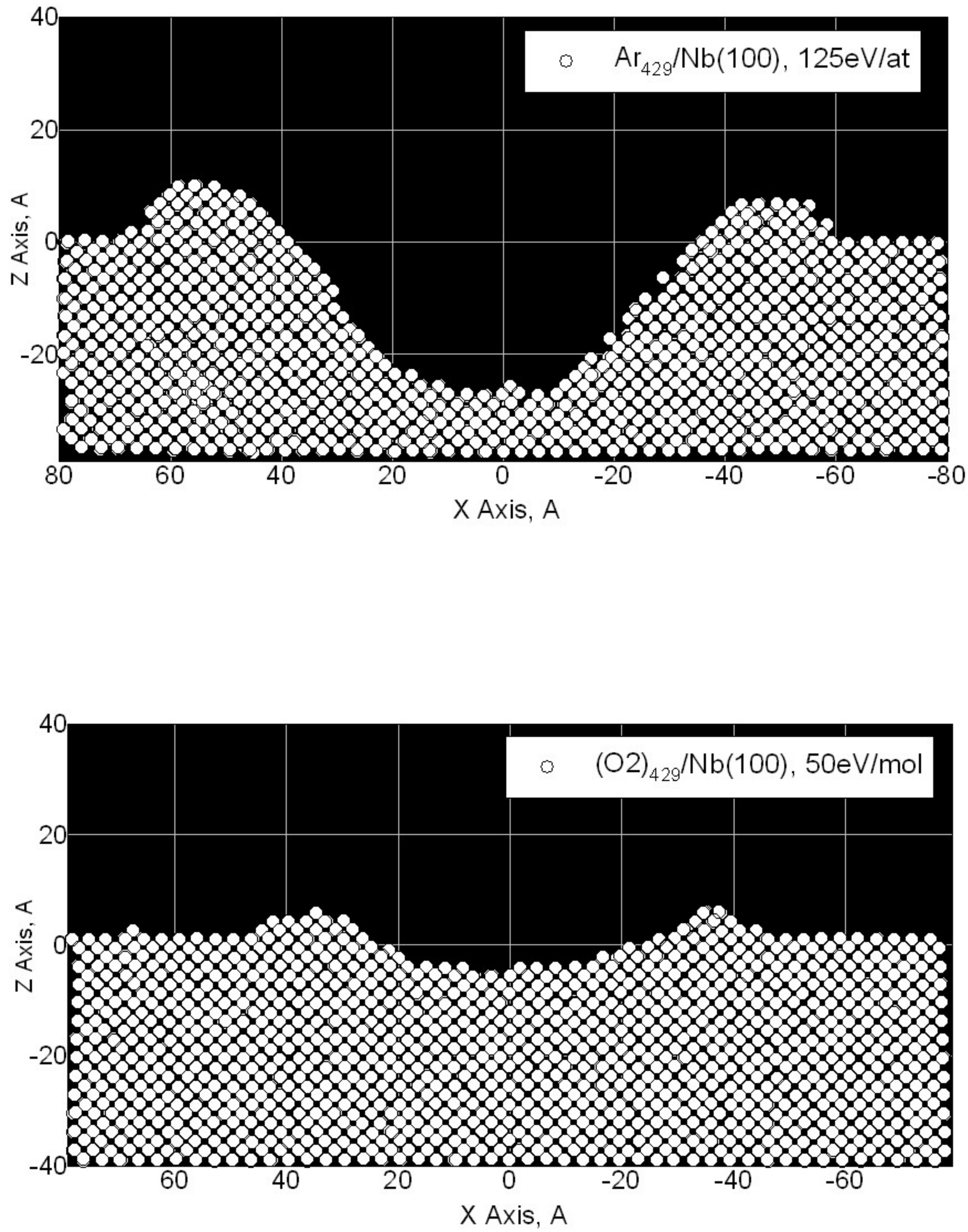

Ar$_{429}$/Nb(100), 125eV/at
Z Axis, A
X Axis, A
40
20
0
-20
80
60
40
20
0
-20
-40
-60
-80
(O2)$_{429}$/Nb(100), 50eV/mol
Z Axis, A
X Axis, A
40
20
0
-20
-40
60
40
20
0
-20
-40
-60

Figure 3

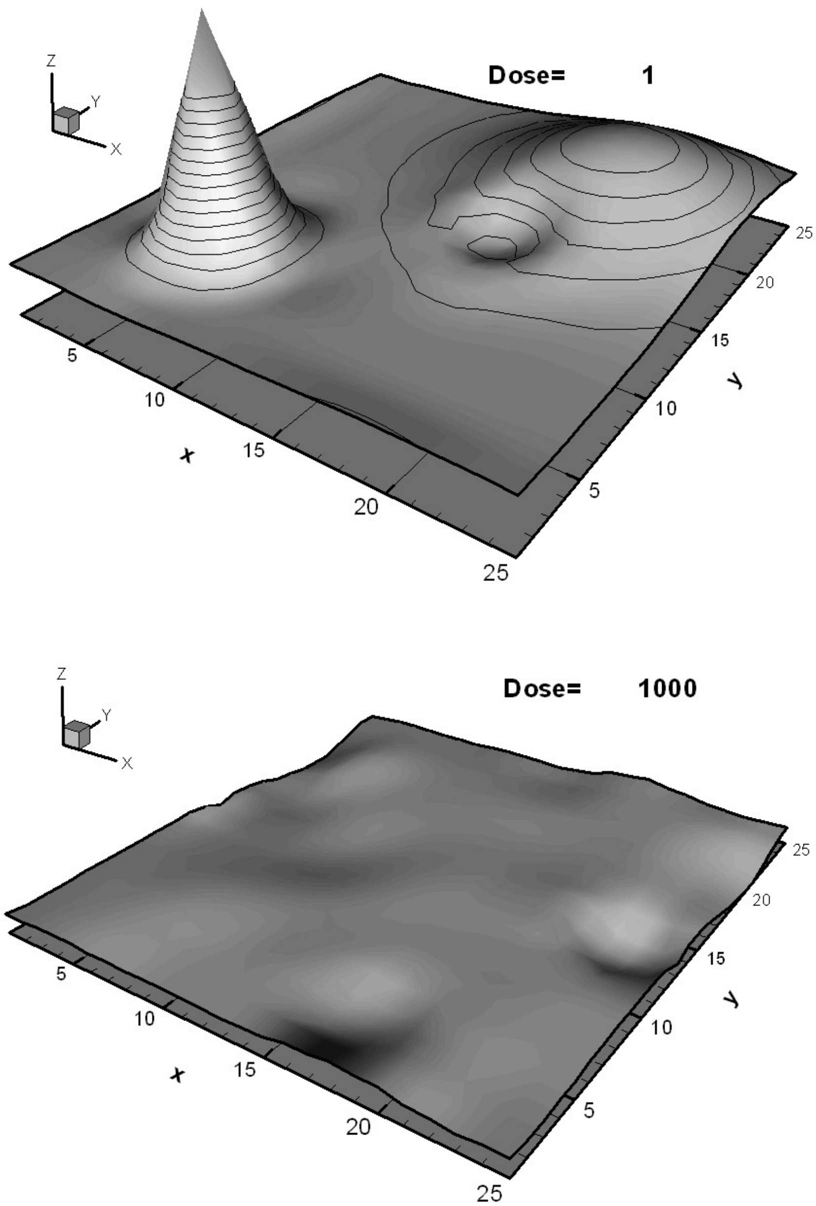
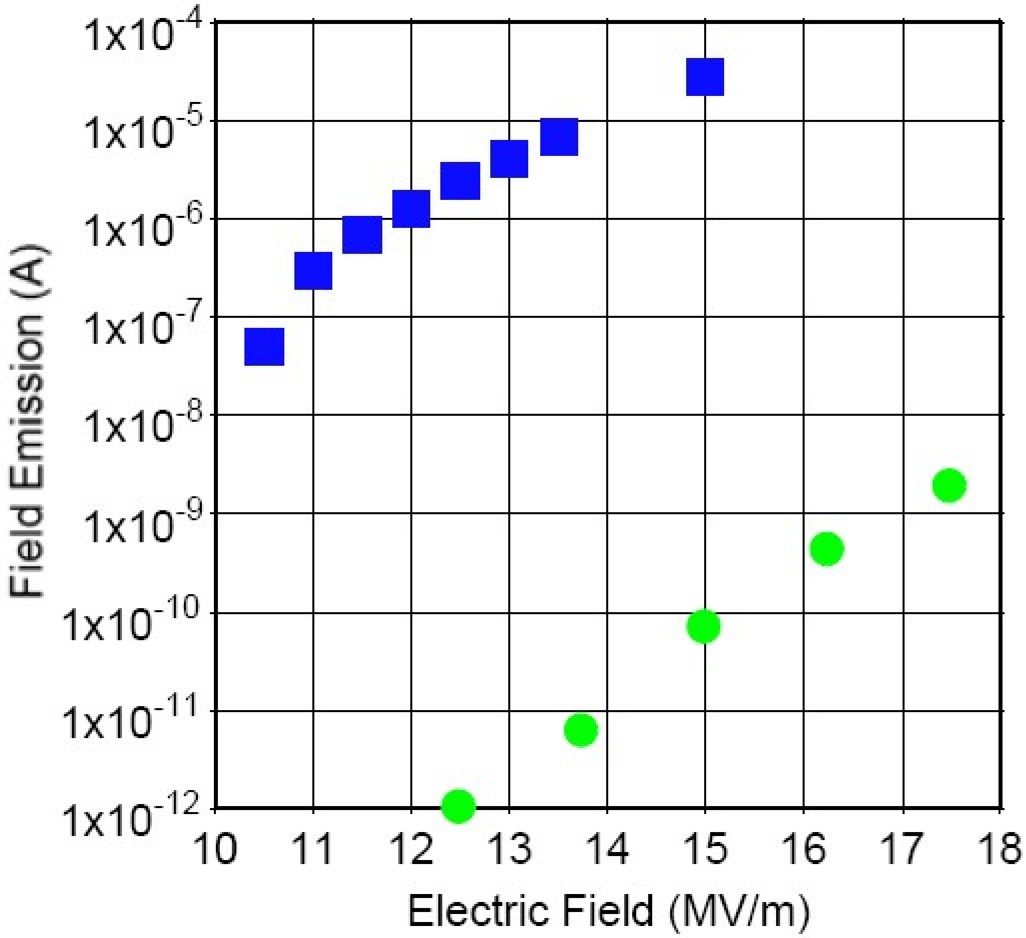


Figure 4



Field Emission (A)
1x10-4
1x10-5
1x10-6
1x10-7
1x10-8
1x10-9
1x10-10
1x10-11
1x10-12
10
11
12
13
14
15
16
17
18
Electric Field (MV/m)

Figure 5

Table 1

Weak Super-conducting Layer Model	The high purity bulk Nb may be covered by a thin (~2 nm) layer of "low-grade" Nb. The critical magnetic field is lower for the "weak" layer. The "weak layer" dissolves into the bulk after baking. The impurity interstitial oxygen, strongly depresses s/c in Nb at several at%
Grain-edge field enhancement model	Grain edges quench at medium field because they reach the critical field earlier due to field enhancement effects; Field enhancement factor distribution consistent with Q-drop at ~20 MV/m needs to peak around 1.4, with narrow sigma
Vortex Penetration Model	The finite nucleation times of Abrikosov vortices allow delaying fluxon penetration beyond the thermo-dynamic critical field, Hc, in a perfect surface (to the so-called "superheating" field)
Wet-dry Oxide Model	Oxides provide localized states to tunneling of the superconductor electron
Hot Spot Model	Q decreases if there is a thermal feedback as the BCS resistance exponentially depends on temperature. Hot spot model: small (mm) "defects" can explain Q-drop (growth by thermal diffusion); The basis of this model is surface non-uniformity
Weak-Link-Model	The strong Q-slope observed in sputtered Nb on Cu cavities is now believed to be in part the result of 100 times smaller grain-size as compared to poly-crystalline, cross-rolled bulk material