THREE-DIMENSIONAL SIMULATIONS OF THE SURFACE TOPOGRAPHY EVOLUTION OF NIOBIUM SUPERCONDUCTING RADIO FREQUENCY CAVITIES

by

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This paper contains results of the three-dimensional simulations of the surface topography evolution of the niobium superconducting radio frequency cavities during isotropic and anisotropic etching modes. The initial rough surface is determined from the experimental power spectral density. The simulation results based on the level set method reveal that the time dependence of the root mean square roughness obeys Family-Viscek scaling law. The growth exponential factors β are determined for both etching modes. Exponential factor for the isotropic etching is 100 times lower than that for the anisotropic etching mode reviling that the isotropic etching is very useful mechanism of the smoothing.

Key words: superconducting radio frequency cavity, niobium, surface modification

INTRODUCTION

Superconducting radio frequency (SRF) cavities have blossomed into the most promising technology for many proposed accelerator-based projects [1]. Various physical and chemical characteristics of the SRF cavity surfaces strongly affect the particle accelerator performances, such as particular the average accelerating field and the cavity quality factor. The extensively used material for construction of SRF cavities is niobium (Nb) which has the highest critical transition temperature, sufficiently high critical field for SRF applications and adequate properties for fabrication. Preparation of cavity walls built of Nb has been recognized as one of the main problems in SRF accelerator technology [2].

Considerable efforts have been devoted in developing of the surface preparation processes that will reduce roughness, allow formation of the surfaces with smaller grain boundaries and lower the level of impurities, embedded in bulk niobium. In preparation of Nb SRF cavities, different techniques are commonly applied to achieve the inner surfaces of cavities smoother with minimal defects and impurities, including buffered chemical polishing (BCP), electropolishing (EP), buffered electropolishing (BEP) and centrifugal barrel polishing (CBP) [2, 3]. The first three involve chemical reactions, while the last one is based on mechanical friction. EP generates a smoother surface than BCP and allows pushing the cavity gradient above 40 MV/m. On the other hand, BEP can produce an order of magnitude smoother surface than that by the EP and is more than 25 and 5 times faster than those of EP and BCP, respectively. Additionally, CBP limits the use of harsh chemicals, which would decrease the environmental impact of the surface treatment process while increasing the smoothness of the surface. Finally, related to the plasma etching, Ar/Cl_2 microwave plasma based processes could also be used for reducing surface roughness and the presence of Nb-oxides and other contaminants that result in the degradation of SRF cavity characteristics [4, 5].

The performance of an SRF cavity is typically described by plotting the resonance quality factor (Q), inversely proportional to the dissipative resistance, *vs.* accelerating gradient. An important class of performance deficit in the push to ever-higher gradient is a decrease in *Q* with increasing gradient – *Q*-drop. Smoothing of the cavity surface includes eliminating both sharp surface features that cause non-field-emitter quenches and small features that contribute to *Q*-drop.

In this paper, we have studied the influence of different etching modes (isotropic and anisotropic) on reduction of the cavity surface roughness. In order to

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simulate a realistic situation, the initial rough surface is generated based on the experimental data for the power spectral density (PSD) curve taken from [6], using the modified convolution method [7]. The etching of this surface is modeled using level set method in the manner similar to that described in [8]. The changes in the surface morphology during different etching modes have been followed in order to obtain complete insight into the smoothing process. The smoothest cavity will have the lowest surface area and thus the lowest total surface resistance.

SIMULATION MODEL

The first element of our simulation model is the artificially produced rough surface that corresponds to an "untreated" Nb surface [6]. The interface width R_q, or root mean square (rms) roughness, that is the rms height of a surface around its mean value, is commonly used to illustrate the rough surface. It is given by $R_q = [(1/N)\sum_{j=1}^{N} h_j^2]^{1/2}$, where N is the number of the scanning points and the heights h_j are measured from the mean line [9, 10]. The value of R_q is strongly dependent on the scan size and the particularities of the area being scanned and it cannot be used to compare data between different types of instrumentation. A surface may seem to be smooth to an instrument with a low lateral resolution with small surface defects that can only be detected by an instrument with a higher lateral resolution. In this situation, one instrument would measure a small roughness parameter, while the other would measure a large roughness parameter on the same surface. Besides, the roughness measurement considers only vertical information; it does not give any information about the lateral topography of surface features. Nevertheless, another statistical characteristic, namely power spectral density (PSD), offers more information about the surface topography [3, 6, 9]. It was recently shown that the PSD based descriptions of surfaces are less dependent on instrumental effects when measuring parameters such as surface roughness and correlation length. Power spectral density (denoted by W in this paper) denotes the spatial-frequency spectrum of surface roughness in inverse-length units. Two-dimensional power spectral density W_2 is a function of the surface heights $h(x, y)$, it represents the squared amplitude of surface features plotted against the spatial frequency of those features, defined as limiting integral form for continuous data sets [11]

$$W_2(f_x, f_y) = \lim_{L \to \infty} \frac{1}{L^2}\left|\int_{-L/2}^{L/2}\int_{-L/2}^{L/2} h(x, y)\,\mathrm{e}^{-2\pi i(f_x x + f_y y)}\,\mathrm{d}x\,\mathrm{d}y\right|^2 \qquad (1)$$

where f_x and f_y are the spatial frequencies of the surface roughness and are related to the lateral dimensions of the surface features and L^2 is the surface area. This function determines the relative contributions of all the spatial frequencies for an ideal measurement of an infinite surface in the limiting case from zero frequency (an infinite surface area) to an infinite frequency (infinitely small area). In real experiments topographic images of surfaces are recorded on finite samples digitizing data in one dimension (at $N N$ points), so one-dimensional PSD $W_1(f_x)$ is defined by periodogram [11, 12]

$$W_1(f_x) = N(m) = \frac{\Delta x}{N}\left|\sum_{n=0}^{N-1} h(x)_n\,\mathrm{e}^{-2\pi i n m/N}\right|^2 K(m) \qquad (2)$$

where $-(N/2) \le m \le (N/2) - 1$, $\Delta x = L/N$ is the spacing between data points in the profile, $h(x)_n$ are the height values of the profile data points $x = nL/N$, and discrete spatial frequency is $f_x = m/L$. $K(m)$ is a factor which equals to 1 except that $K(\pm N/2) = 1/2$ at the ends of the power spectrum. A window is often inserted in the summation in order to condition the profile data and eliminate spurious effects caused by non-zero terms at the end points. Spectral estimation from real data is limited by the bandwidth limits, aliasing, trending, and statistical instability. Real data are recorded over a finite length and sampled at a finite interval so reliable spectral estimates can only be performed over a limited range of surface frequencies

$$\frac{1}{L} \le f \le \frac{N}{2L} \qquad (3)$$

which means that the minimum spatial frequency is limited by the recorded length, while the maximum is limited by the half of the sampling interval-Nyquist frequency.

Two-dimensional PSD W_2 is necessary to generate initial rough surface, but the measurements provide only one-dimensional function W_1. The general relationship between the one-dimensional (2) and two-dimensional (1) power spectral densities is given by

$$W_1(f_x) = \int_{-\infty}^{\infty} \mathrm{d}f_y\, W_2(f_x, f_y) \qquad (4)$$

If two-dimensional spectral density W_2 is known; it is relatively easy to obtain one-dimensional W_1. The inverse, however, is not possible in general case, except for an extreme anisotropic and an isotropic surface [13]. If we assume that the surface is isotropic, *i. e.*, $f^2 = f_x^2 + f_y^2$ eq. (4) can be re-written in the form

$$W_1(f) = 2\int_f^{\infty} \frac{f'\mathrm{d}f'}{\sqrt{f'^2 - f^2}} W_2(f') \qquad (5)$$

In this case, the required link between W_2 and W_1 is the inverse Abel transform

$$W_2(f) = -\frac{1}{\pi}\int_f^{\infty} \frac{\mathrm{d}f'}{\sqrt{f'^2 - f^2}} \frac{\mathrm{d}}{\mathrm{d}f'} W_1(f') \qquad (6)$$

Since the measured PSD W_1 is limited on the upper side by the Nyquist frequency, in order to accomplish the integration from f to ∞ in eq. (6), in actual calculation we extrapolated W_1 by an analytical expression, as it is described in [13].

In this way obtained two-dimensional PSD W_2 is used to generate initial random rough surface that corresponds to the experimentally measured one-dimensional PSD W_1. Here the modified convolution algorithm described in details in [7] is used. The evolution of this surface during the etching process, which is the main objective of this paper, is simulated using the level set method [14].

The level set method is a highly robust and accurate computational technique for tracking interface surfaces by representing a surface using an auxiliary function $\varphi(x, t)$ at a certain time t, called the level set function. The initial surface is represented as the zero level set of the function and its time evolution is caused by forces or fluxes of particles reaching the surface in the case of the etching process. The velocity of a point on the surface normal to the surface will be denoted by $R(x, t)$, and is called the velocity function. For the points on the surface this function is determined by physical models of the ongoing processes, in the case of etching by the fluxes of incident particles and subsequent surface reactions. The time evolution of the level set function is described by the Hamilton-Jacobi equation [14]. The simulation results presented here are obtained using our three-dimensional simulation package based on the sparse field method [15] for solving level set equations. In these simulations the surface velocity function $R(x, t)$ for isotropic or anisotropic etching was modeled by simple analytical relations. In the case of the isotropic etching the dependence of the surface velocity on the incident angle is described by the expression $R = R_0$ (isotropic in all directions). The velocity functions $R = R_0\cos(\theta)$ corresponds to the ideally anisotropic etching where represents the angle between the normal to the surface and the direction of the incoming particles. Actually, in the real etching processes both modes are present. Although these are the simplest forms of angular dependences, they describe the anisotropic etching process quite correctly. The physical sputtering mechanism, which usually has a significant contribution to the plasma etching of semiconductors, can be neglected in the case of niobium surfaces [5].

RESULTS AND DISCUSSION

The initial surface (100 µm × 100 µm) determined from the one-dimensional PSD $W_1(f)$ taken from fig. 6 in ref. [6] relating to an "untreated" Nb surface is shown (as inset) in fig. 1 together with $W_1(f)$. The rms roughness of this surface is $R_q \sim 1$ µm, but it is scaled with factor 5, in order to be noticeable in the figure.

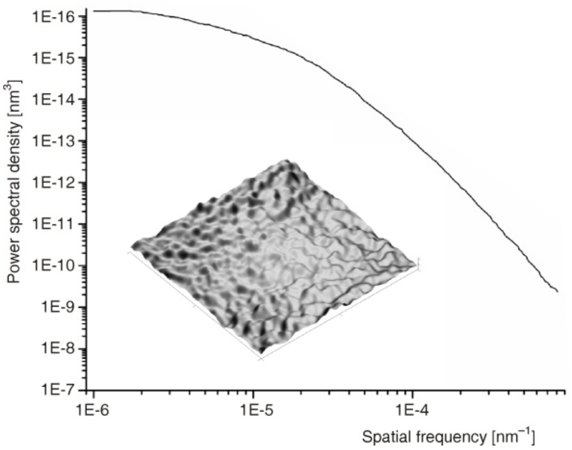

Figure 1. Experimental power spectral density (PSD) taken from ref. [6]. The initial rough surface (100 µm 100 µm) is in inset

The pictures below display the time evolution of the initial surface achieved by our level set simulation package based on the sparse field method for solving three-dimensional level set equations that describe the morphological surface evolution during etching process. The etching of Nb surface in Ar/Cl$_2$ plasma is dominantly of chemical nature, meaning that the etching rate is determined by the concentration of reactive species in the plasma and that the etching rate is isotropic $R = R_0$. The three-step etching process, described in [5], comprised a cleaning step, a fast removal step, and a smoothening step. The first step performed in pure argon is not of interest for the present analysis. The second, fast removal step, is characterized by high etching rate and significantly reduces influence on the surface roughness. The smoothening step is very effective in reducing roughness, at the expense of lower etching rate. In fig. 2. the time evolution of initial surface (shown in fig. 1.) during anisotropic etching pro-

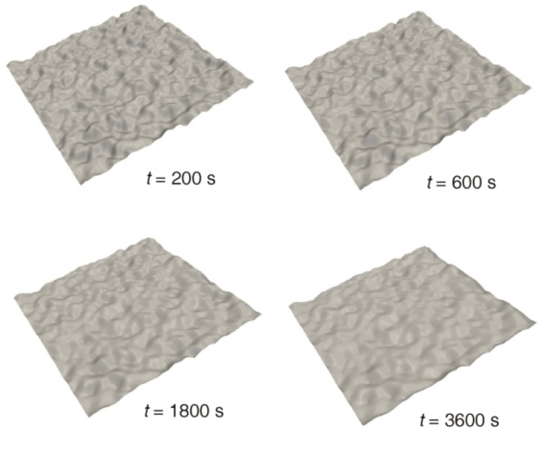

Figure 2. The time evolution of the initially rough surface induced by anisotropic plasma etching ($R = R_0 \cos\theta$ with $R_0 = 1$ µm/min)

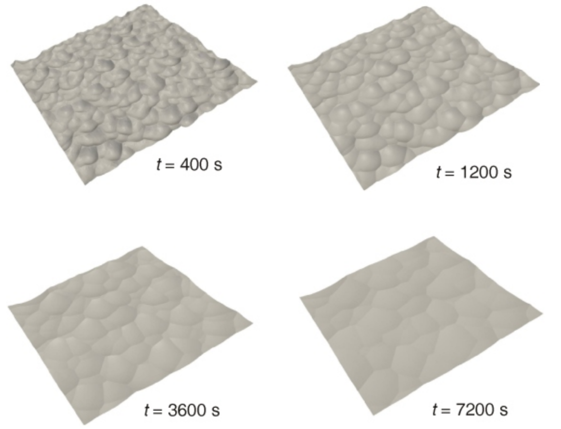

Figure 3. The time evolution of the initially rough surface induced by isotropic etching (R = 0.5 μm/min)

cess is shown. The etching rate is taken to be $R = R_0\cos\theta$, with R_0 = 1 μm/min in accordance with [5]. Obviously, the anisotropic process does not reduce roughness significantly. The time evolution during isotropic process is presented in fig. 3. The etching rate is taken to be lower, R = 0.5 μm/min, but the surface roughness is efficiently reduced. Besides, the obtained surface topography is very similar to some of experimental plasma-treated samples (see fig. 9. in [4]).

Simulation results, presented here, are in accordance with the previously published results [8] which confirmed that the isotropic etching mode smoothests surfaces successfully, while the anisotropic process is much less effective, which is in line with the simulation results shown here [8]. When the etching is isotropic all surface elements are etched away with the same etch rate R_0, though in the anisotropic case the surface elements inclined to the horizontal plane are etched with the rates proportional to $R_0\cos\theta$, that is smaller than R_0. As a result the smoothing by anisotropic etching process is significantly slower, as can be seen from figs. 2. and 3.

The dynamics of smoothing process *i. e.*, the time dependence of rms roughness R_q is presented in fig. 4. In both etching modes, R_q decreases with the etching time following t^β Family-Viscek scaling law [16], where the growth exponents β are different for isotropic and anisotropic case.

CONCLUSIONS

In this paper the sparse field method for solving three-dimensional level set equations that describe the smoothing of the initially rough niobium surface is applied. The initial rough surface is created from the experimental one-dimensional PSD function. The two-dimensional PSD, necessary for surface formation, is reconstructed from one-dimensional PDS, under the assumption of isotropy. For both etching modes, the rms roughness decreases with the etching time following t^β scaling law. The exponential factor for the isotropic etching is 100 times lower than that for the anisotropic etching mode. The simulation results shown here, confirm that the surface roughness could be reduced by the isotropic etching, while the anisotropic etching is not an effective mechanism of smoothing, which is in accordance with the experimental data. Unfortunately, there are no measurements that describe the PSD before and after the plasma etching process, so we were not able to compare our simulation results with them. Simulation results, presented here, can be used in order to optimize the parameters of the etching processes required in generating the high quality niobium surfaces for superconducting radio frequency cavities.

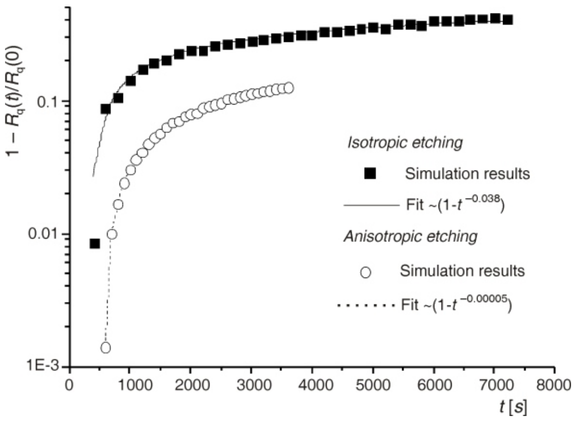

Figure 4. The time dependence of the rms roughness during the isotropic and anisotropic etching. Simulation results are presented by symbols, while lines show fits to the simulation data

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AUTHOR CONTRIBUTIONS

Theoretical analysis, coding, and simulations were carried out by B. M. Radjenović and M. D. Radmilović-Radjenović. The coding and simulation of the initial roughness of niobium surface was carried out by P. D. Beličev. The manuscript was written by M. D. Radmilović-Radjenović, B. M. Radjenović, and P. D. Beličev. The figures were prepared by B. M. Radjenović.

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ТРОДИМЕНЗИОНАЛНЕ СИМУЛАЦИЈЕ ПОВРШИНСКЕ ТОПОГРАФИЈЕ НИОБИЈУМСКИХ СУПЕРПРОВОДНИХ РАДИО-ФРЕКВЕНТНИХ ШУПЉИНА

Рад садржи резултате тродимензионалних симулација еволуције површине суперпроводних радио-фреквентних шупљина од ниобијума током изотропног и анизотропног процеса нагризања. Почетна површина одређена је из експериментално добијене спектралне густине снаге. Резултати симулације засновани на методи ниво скупова показују да временска зависност средњег квадратног одступања храпавости површина задовољава *Family-Viscek*-ов закон скалирања. Фактори експоненцијалног раста одређени су за оба мода процеса нагризања потврђујући да је изотропно нагризање много ефикаснији механизам равнања површина. Овде представљени резултати симулација, могу се користити за оптимизацију параметара процеса нагризања који су неопходни у генерисању површина од ниобијума високог квалитета за суперпроводне радио-фреквентне шупљине.

Кључне речи: суйерйроводна радио-фреквенйна шуйљина, ниобијум, модфикација йовршине