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VACANCY-HYDROGEN DYNAMICS AND MAGNETIC IMPURITIES DURING MID-T BAKE

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Abstract

Positron annihilation measurements allow to study the hydrogen interaction with vacancies in a crystal lattice. Furthermore, the $3\gamma/2\gamma$ ratio of the positronium annihilation showed local magnetic impurities in the native niobium-oxide layers. Dynamic studies of these properties in annealing studies up to 300° C will be presented. The discussion is accompanied by X-ray reflectivity studies performed on single crystal samples to study the niobium oxide dissolution and structural reorganization. The dynamics of magnetic impurities during a Mid-T bake will be presented, put into the context of cavity studies and a potential link to rf properties will be presented.

INTRODUCTION

Annealing procedures to tailor the chemical composition of superconducting radio-frequency (SRF) cavities made out of niobium have been applied for decades. But only recently, a 300 – 400° C anneal for 3 h in UHV was studied (the newly dubbed "Mid-T Bake") and showed very high quality factors of $Q_0 \approx 5 \times 10^{10}$ at already 2 K [1]. In addition, a behavior called "anti-Q-slope", a positive slope in the Q_0 vs. applied accelerating field E_{acc} representation, was observed. This behavior was only observed on doped cavities so far [2, 3]. As been reported by He et al. and Ito et al [4, 5], this anneal was successfully reproduced at other labs rather fast, even relaxing the annealing conditions (using furnaces and cavities with caps rather than in-situ annealing of cavities while still under vacuum as been done by Posen et al.). Similar studies were pursued by Palmer et al. [6], in which observations in agreement with the recent Mid-T bake were already described (increase of the sensitivity to ambient magnetic field, reduction of the critical temperature, decrease of the BCS resistance).
In this paper, we will present the results of the first application of the Mid-T bake in the industry and discuss another similarity of the Mid-T bake with the doping procedure, besides the anti-Q-slope. Furthermore, we will show that a reorganization of a lower niobium-oxide, NbO, takes place at 300° C which has a significant impact on the overall properties of the near-surface region and its interfaces of the niobum rf surface.

CAVITY STUDIES

Four 1.3 GHz single-cell cavities were sent for a 300° C anneal for 3 h to Zanon R.I.. Each cavity underwent a baseline rf test before shipment. The standard surface preparation was applied, but two cavities got a final electropolishing (EP) as last treatment step (namely 1DE9 and 1AC2), while the other two cavities underwent a subsequent low-temperature anneal, the so called 120° C bake, as last treatment step (namely 1DE5 and 1DE7). The decision was, that one of each cavities with the different final surface treatment were annealed together in one furnace run. The first furnace run (cavities 1AC2 and 1DE7) was done without caps installed, while the second run (cavities 1DE9 and 1DE5) was done with caps installed. Up to now, only the cavities from the first furnace run were tested, and the rf tests at 2 K before and after the treatment are shown for 1AC2 in Fig. 1 and for 1DE7 in Fig. 2. Besides the shown test results, R_s

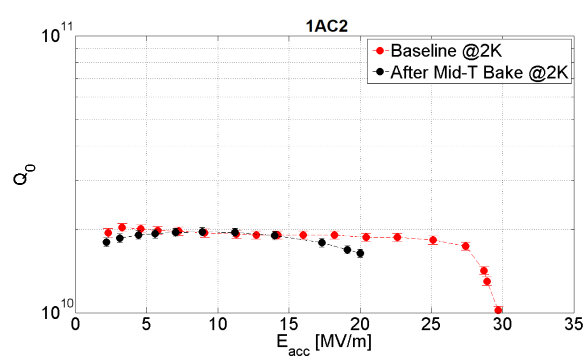

Figure 1: Quality factor versus applied accelerating field for 1AC2 at 2 K. The measurement before (red) and after (black) the Mid-T bake is shown. An anti-Q-slope is not observed. The cavity is quench limited without field emission.

versus temperature measurements were done. The residual resistance R_{res} of 1AC2 increased from 1.9 nΩ before the treatment to 8.5 nΩ after the treatment. The residual resis-

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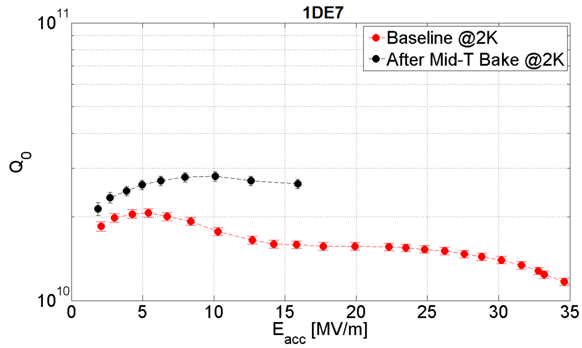

Figure 2: Quality factor versus applied accelerating field for 1DE7 at 2 K. The measurement before (red) and after (black) the Mid-T bake is shown. An anti-Q-slope is observed. The cavity is quench limited without field emission.

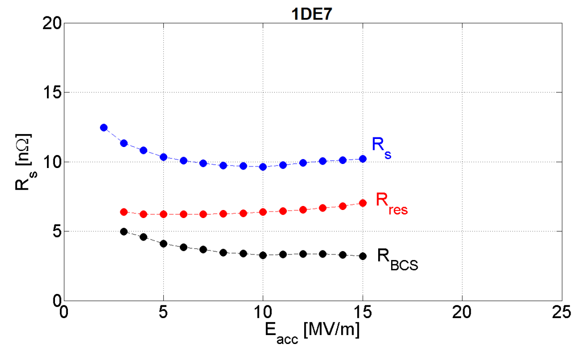

Figure 4: Surface resistance versus applied accelerating field for 1DE7 at 2 K. The surface resistance R_s is decomposed in its contributions of the residual resistance R_{res} and the BCS-term R_{BCS}. The anti-Q-slope in the R_{BCS} is observed.

tance R_{res} of 1DE7 remained nearly unchanged with 5.5 nΩ before the treatment to 5.1 nΩ after the treatment. For 1AC2 the ratio of the superconducting gap Δ normalized to the Boltzmann constant $\frac{\Delta}{k_b}$ was found to be increased to 19.95 compared to 17.65 before, and for 1DE7 to be 20.06 after the Mid-T bake compared to 17.43 before.

A decomposition of the surface resistance in its both contributions R_{res} and the BCS-term R_{BCS} as a function of the applied accelerating field, shown in Figs. 3 and 4, allowed a more detailed discussion of the rf behavior. Surprisingly, the R_{BCS} term behaves as expected from lab-results elsewhere after the Mid-T bake: its value is below 6 nΩ and increases with increasing accelerating field thus being responsible for the observed anti-Q-slope. It is the residual resistance, which did not improve for 1DE7 and even increased for 1AC2, which prevents the high quality factors as shown for this treatment.

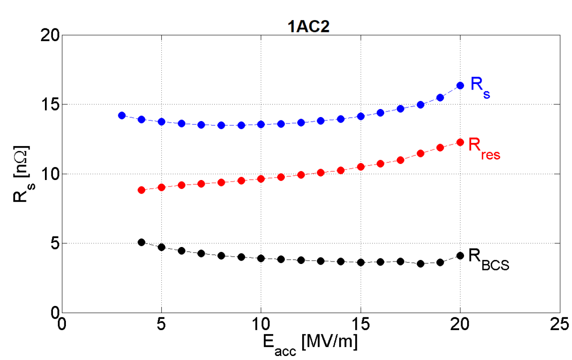

Figure 3: Surface resistance versus applied accelerating field for 1AC2 at 2 K. The surface resistance R_s is decomposed in its contributions of the residual resistance R_{res} and the BCS-term R_{BCS}. The anti-Q-slope in the R_{BCS} is observed.

Another surprising result is the occurrence of a local minimum or "dip" in the frequency versus temperature measurements done for those cavities. Figure 5 shows the frequency change as a function of the cavity temperature for 1AC2. The behavior before the treatment (red curve) is explained by the Meissner-effect, causing an expulsion of the electromagnetic field, decreasing the resonating volume and hence slightly increasing the frequency. A local minimum below the critical temperature T_c, such as evident for the Mid-T bake, cannot be explained in such a simple model. Such a dip was only recently shown to occur for doped cavities as well [7].

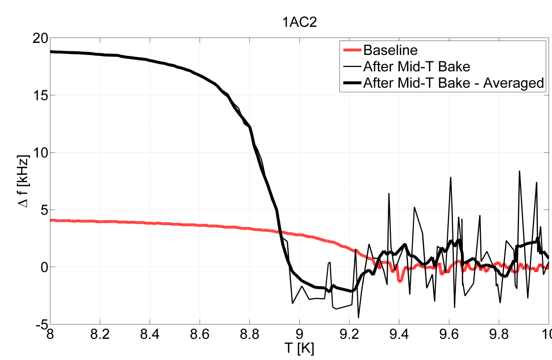

Figure 5: Frequency change versus cavity temperature, relative to the frequency above T_c. The measurement of 1AC2 before (red) and after (black) the Mid-T bake is shown. A dip below T_c after the Mid-T bake appears and a significant frequency change compared to the convential treatment is obvious.

Although two more cavity tests are pending and an increase in statistics is necessary, summarizing the results so far, allows the conclusion that the first industrial application of the Mid-T bake shows an at least partially successful treatment: a reduction of the R_{BCS} contribution and the anti-Q-slope development and the occurrence of the local minimum below T_c. Still, two questions remain: (i) what is the origin of the dip in the frequency versus temperature measurement and (ii) why did the residual resistance R_{res} not improve as expected?

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MATERIAL STUDIES

The development of the native niobium-oxide layer while annealing in UHV conditions is well known, and has been studied using different methods, see e.g. [8, 9]. Figure 6 shows the x-ray reflectivity (XRR) measurements of the layer for four different temperatures. X-ray diffraction measurements from Semione et al. showed the increase of the interstitial oxygen concentration in the niobium lattice as a consequence of the dissolution of the Nb_2O_5-layer up to 250° C. Recent parameter studies on samples baked with

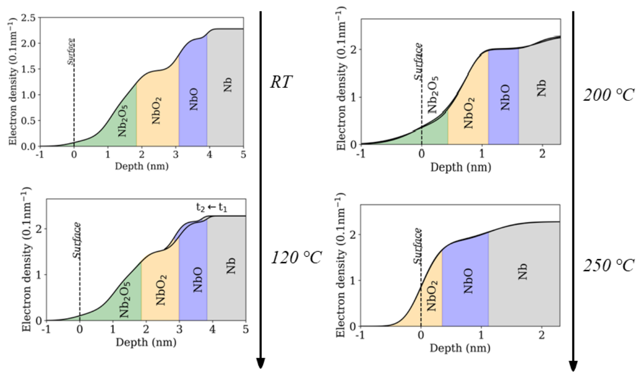

Figure 6: Electron-density profiles obtained from the fits of XRR measurements. The measurement collected data from RT up to 250° C. The complete dissolution of the Nb_2O_5-layer is observed at 250° C.

temperature and duration variations intended to investigate the Mid-T bake align with those findings [10]. But besides the chemical composition, structural properties are of major importance for the understanding of the Mid-T bake.
Niobium is arranged in a bcc lattice, while the first oxide-layer on top, NbO, builds in an fcc arrangement. This causes a misalignment when stacking those two unit-cells onto each other. Depending on the atomic radius of the participating elements, the layer thickness, lattice orientation and deformation and growth temperature, energetic optimal misalignment angles exist and for fcc - bcc interfaces, three orientations are predicted by the rigid-lattice theory and observed for many metal on metal systems. E.g., for Nb(100) the optimal in-plane relation to the NbO(110) cell, shown in Fig. 7, results in a tilt of 5.26 degrees between the rows of $[101]_{fcc}$ w.r.t. $[001]_{bcc}$ [8, 11–13]. Measurements conducted by Delheusy et al. [8] show that the in-plane orientation of this interface for regular niobium used for SRF applications does not show the optimal relation, see Fig. 8: neither is the oxide fully structured, nor is the orientation close to the optimal angle. An annealing of the surface at 145° C in UHV causes an increase of the diffraction intensity, meaning an increased structure of the interface, which is still not optimal. Only an anneal at a temperature of 300° C provides enough thermal energy that the interface reorganizes itself in a way, such that it aligns closer to the theoretical optimum.
In addition, the out-of-plane properties also show an interesting ordering affect. It is known that the structural and

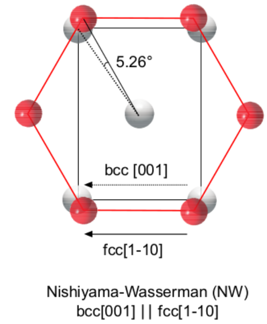

Figure 7: Possible in-plane orientation relationships at the fcc(111)/bcc(110) interface based on the rigid-lattice model.

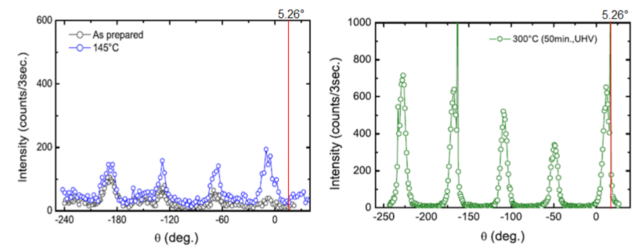

Figure 8: Diffracted intensity as a function of the in-plane rotation angle θ for different thermal treatments (RT - black, 145° C - blue, 300° C - green) applied on the Nb(110). In all scans the sixfold symmetry of the NbO(111) planes is observed. Image taken from [8].

electrical properties of niobium oxides depend on the substrate properties [14], and that interface and subsurface oxygen can act as precursor for the formation of NbO [15]. At 300° C, Delheusy et al. showed that an interstitial oxygen ordering occurs and the lattice transition changes by creating an intermediate Nb_2O-layer as a buffer between the Nb and NbO lattice.
An important consequence of the reduction of the lattice mismatch is, that the vacancy concentration in the niobium-oxide has to decrease as well. Hence, we studied the vacancy-dynamics in the near-surface region and the given temperature range using positron-spectroscopy. The advantages of positron-spectroscopy for this kind of research and first results were reported elsewhere [16], and we intend to focus on the so-called "$3\gamma/2\gamma$ ratio" for this discussion. While radiating metals with positrons, not only direct annihilation takes place, but also the formation of short-lived e^+e^--bound states called positronium. Depending on the orientation of the spins of the particles in the bound state, the positronium will decay in two or three photons, due to angular momentum conservation. The decay in three photons can be suppressed if the corresponding positronium is in a magnetic field causing a spin-flip, and hence changes to the lower-energetic state which decays into two photons. Therefore, the "$3\gamma/2\gamma$ ratio" is sensitive to magnetic ordering in the vicinity of vacancies. Figure 9 shows the measurement of this ratio as a function of time and for the first 5 nm, and each measurement is for a different annealing temperature. As expected

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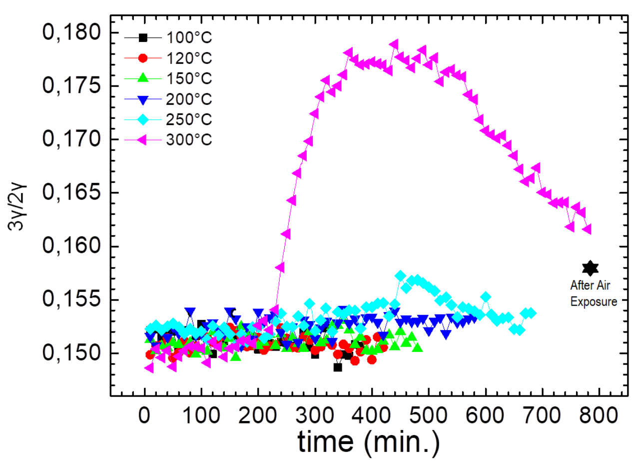

Figure 9: $3\gamma/2\gamma$ ratio vs. annealing time at a fixed positron energy of 1.5 keV ($\approx$ 5 nm) for various annealing temperatures. The annealing temperature was reached after a ramping of 1° C per second and held for 4h. The last data point of each curve is after cooldown at room temperature. The black datapoint shows the measurement of the sample after air exposure subsequent to the 300° C anneal.

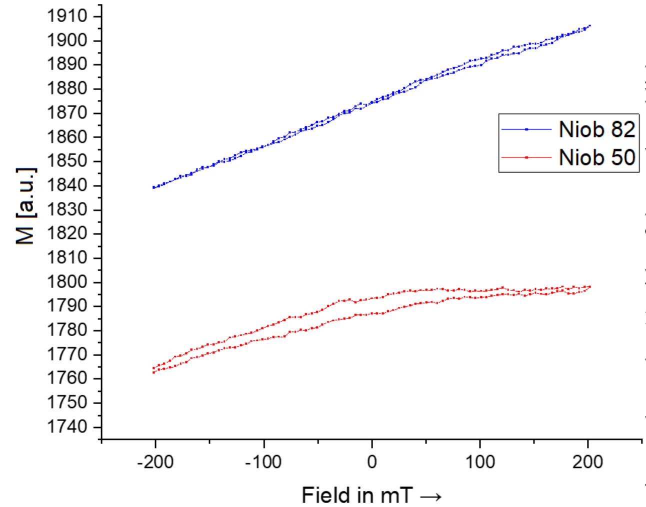

Figure 10: Magnetization as a function of applied field. The magnetization is encoded in the gray values of the Kerr-microscope images. The offset is influenced by the surface roughness. Sample 50 (EP+120° C) shows ferromagnetic behavior, while sample 82 (EP+120° C N-Infusion) behaves paramagnetic.

from the reorganization of the NbO-Nb interface, at 300° C the ratio increases considerably, which remains after cooling down and even after the sample was exposed to air. From this measurement, a decrease of magnetic moments can be deduced. The location of those magnetic moments is not in the Nb_2O_5-layer, since this was already dissolved at 300° C. Still, the reduction of the ratio after exposure to air can be explained by the regrowth of the niobium-pentoxide. The concept of magnetic impurities are not new in SRF and a correlation with RF behavior was shown already by Proslier et al. [17, 18], while there it was assumed that the niobium-pentoxide layer is the dominating contribution. The cause of those magnetic impurities are localized magnetic moments, e.g. missing oxygen atoms creating vacancies which then act as donors [19–21].

Another consequence of those magnetic impurities might be the "unexpected ferromagnetic behavior of dielectric oxides" [19]. To test the conclusion of magnetic impurities, samples with different surface treatments were inspected with a Kerr-microscope. This technique is rather surface sensitive, with a max. penetration depth of 50 nm and can spatially resolve the magnetization of surfaces as a function of the applied magnetic field. Our preliminary results are shown in Fig. 10. In agreement with the magnetic impurity model, deduced from the $3\gamma/2\gamma$ ratio, the niobium surface which underwent the standard surface preparation shows a weak ferromagnetic behavior. Compared to that, a sample which underwent a different final treatment, the so-called nitrogen infusion [22], shows a paramagnetic behavior, as it could be expected from niobium. The vanishing ferromagnetic behavior of infused samples can be explained by the magnetic coupling between those impurities, which become weaker when hydrogen-hydrogen distance increases [23].

Concluding the material studies shown here, it was shown that during an 300° C anneal, the Nb-NbO-interface reorganizes itself to reduce the lattice mismatch, which reduces the vacancy concentration in the oxide-layer, which act as magnetic impurities. At the same time, an increase and reordering of the interstitial oxygen takes place. The reorganized oxygen causes the formation of an intermediate Nb_2O-layer to form a smoother transition from the bcc to the fcc lattice.

RELATION TO RF BEHAVIOR

Equipped with the findings above, a discussion of the two questions from our cavity studies can now be done: (i) what is the origin of the dip in the frequency versus temperature measurement and (ii) why did the residual resistance R_{res} not improve as expected?

Origin of the dip?

As has been pointed out by Bafia et al., a current redistribution model such as suggested by Barra et al. can explain the local minimum in the frequency versus temperature measurement [24]. This model assumes regions, with a critical temperature below that of niobium, in the vicinity of the surface. Once the cavity crosses the critical temperature of niobium, the current is expelled from regions farther away than the temperature dependent effective London penetration depth. Regions with a lower critical temperature than niobium will stay normal conducting and will effectively be shielded from the current. If those regions are in the near-surface region, the current will be redistributed and "pushed" deeper into the material. Once the critical temperature of those regions is reached, the current can flow close

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to the surface again, and the simple model of the shrinking resonator volume can be applied. Such regions can be found for doped cavities, since β-Nb_2N has been observed on the surface of individual grains even after a surface removal of 5 μm [25]. For the Mid-T bake no such regions have been identified so far, but it is well known that an oxygen concentration increase of 1 at.% can reduce the critical temperature of niobium by 1 K. Given the strong lattice orientation dependency of local diffusion and reorganization processes, an inhomogeneous distribution of the oxygen concentration can be expected, and the order of magnitude of this inhomogeneity might be enough to cause such a behavior. Another observation of the frequency vs. temperature measurement is the rather strong frequency change compared to the conventional treatments which can also be explained by the formation of the intermediate layer. As it has been observed in [26], the reorganization is taking place in the NbO-layer, and the formation of the Nb_2O-layer is well contained to the near-surface region and no inward-diffusion of oxygen appears. And as it has been shown above, the oxygen diffuses away from the surface at 250^o C, and with the lack of further oxygen coming from the oxide-layer, a general reduction of the oxygen-concentration in the near-surface region is the consequence, which implies an increase of the mean free path. An increase of the mean free path leads to a general decrease of the penetration depth, making the flux-expulsion more effective compared to the conventional treatments, and hence leads to a higher frequency of the cavity.

Development of R_{res}?

The residual resistance of 1AC2 increased by about more than a factor of 4 due to the Mid-T bake, while the residual resistance for 1DE7 remained unchanged. The deviation from the expected behavior of the resistance alone is worth to discuss, but what else is surprising, is that both cavities were put together in the same furnace run and still showed different results. From material studies, we know that the oxide-layer evolution depends on the substrate properties and that the oxygen pressure in the furnace has a significant impact on the actual formation. The residual gas analysis of the furnace run showed a significant partial pressure of O_2 during the 300^o C anneal. It is known that the Nb_2O_5-layer will not dissolve at elevated temperature if oxygen is provided, and can even grow at the expense of the underlying NbO_2-layer [8, 9, 14, 27]. Hence, the oxide-layer reorganization didn't take place "as it should". At the same time, the difference between 1DE7 and 1AC2 can be explained by the additional 120^o C anneal which 1DE7 had. As it was shown above in Fig. 8 and was also discussed, a first ordering of the layer is visible at 145^o C. Hence, it is reasonable to assume that 1DE7 was more robust against a deviation from the annealing parameters, since a first "seed" of the needed reorganization already took place, explaining why for 1DE7 the residual resistance remain unchanged, instead of increased as for 1AC7.

How can the Mid-T bake affect the rf performance?

Ma et al. [26] annealed niobium samples and came to the same observations as Delheusy et al. or Semione et al., that the Nb_2O_5-layer dissolves around 270^o C and that the Nb_2O-layer forms. Furthermore, the density of states (DOS) of those layers were measured and it was observed that the reorganization and formation of the Nb_2O-layer is accompanied by a redistribution of states in the valence-band [26]. This is in agreement with the increased ratio $\frac{\Delta}{k_b}$ after the Mid-T bake, which changed drastically due to the treatment. This is a direct implication of the Mid-T bake, altering the DOS compared to the regular surface treatments. Furthermore, in [14] it was shown that the regrown Nb_2O_5-layer after oxidation in air will vary in its dielectric properties, such as the semiconducting gap, based on the properties of the underlying niobium oxides.

Another impact on the DOS are the magnetic impurities. As has been shown in [18], a correlation between rf induced losses and the existence of the magnetic impurities was found. Accompanying theoretical work showed that a inherent non-zero residual resistance is a consequence of magnetic impurities in the rf surface [28], and a consequence in general for any existing sub-gap states regardless of the microscopic origin. A more recent approach by Kubo et al. discusses different realistic surfaces [29], including sub-gap states and magnetic impurities in the material, further showing their potential to minimize rf losses and modify the dynamic loss mechanisms.

In addition, the formation of niobium-hydrides while cooling down to the operational temperature of 2 K have been identified as a significant loss mechanism during the operation of rf cavities [30] and the hydrogen trapping potential of interstitial nitrogen and oxygen is well known [31]. As has been pointed out already, this can lead to a mitigation of the formation of hydrides, further reducing the surface resistance [32].

CONCLUSION

In this work, the rf tests of two cavities after the first industrial Mid-T bake shows an at least partially successful treatment: a reduction of the R_{BCS} contribution and the anti-Q-slope development and the occurrence of the local minimum below T_c, but the expected reduction of the residual resistance was not observed. This can be explained by an increased oxygen partial pressure during the furnace run, preventing the oxide-layer reorganization causing the improved rf performance of the Mid-T bake. The appearance of a local minimum in the frequency versus temperature after the Mid-T bake, sharing this effect with doped cavities, can be understood in terms of a surface current redistribution due to regions with a critical temperature below that of niobium.

The material studies presented here can explain why 300^o C is a threshold temperature for the niobium rf surface, and an anneal at that temperature has a variety of effects on the DOS of niobium and a prominent loss-mechanism.

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