ELECTRO- AND CHEMICAL- POLISHING NB CAVITIES

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Abstract

Standard treatments to achieve excellent high rf power Nb accelerator cavities include electro polishing (EP), buffered chemical polishing (BCP), and ~120°C UHV baking (LTB). Those treatments change for RRR>100 Nb: rf residual losses R_{res}, BCS rf losses $R_{BCS}(T)$, low field Q- (LFQ), medium field- (MFQ) or high field- (HFQ) Q slope. Those differences between BCP, EP and LTB are related to differences in oxidation where Nb_2O_5 grows on Nb, O^{2-} is drawn through the double layer and through Nb_2O_5 injecting O into the open Nb lattice nucleating Nb_2O_5 crystallites straining the NbO_x/Nb interface heavily worked out below which gives the first consistent explanation for the superiority of EP over BCP and the reasoning for the advantage of LTB. For example by EP and LTB strong O built up and O precipitation at Nb surfaces is found being demonstrated by H_{c3} increases and by HFQ reductions. By BCP the repeated Nb_2O_5 crystallite growth creates dislocations and injects O into larger Nb depth enforcing weak link (WL) growth, i.e. R_{res}, MFQ and HFQ are enforced.

INTRODUCTION

Standard treatments to achieve excellent high rf power Nb accelerator cavities are: high pressure water rinsing (HPR), electro polishing (EP) more than 50µm Nb, buffered chemical polishing (BCP) more than 100µm Nb, and ~120°C UHV baking (LTB) [1-5], which change the rf residual losses R_{res}, the BCS rf losses R_{BCS}, the low field Q-drop (LFQ), the medium field Q-drop (MFQ), the high field Q-drop (HFQ), the impedances $Z(T>T_c, \omega<MHz, B_{dc})$ up to depth of 50µm and the ratio $H_{c3}/H_{c2}=r_{32}>1.69$. BCP, EP and LTB mainly differ in details of the oxide removal and the oxidation process, especially in strain relaxation and O precipitation, being summarized below.

The quality factor $Q_0=G/R$ is given by G^H containing the current distribution and R^H containing material properties

$$R^H(T,\omega,H)=R^H_{res}(\omega,H)+R_{BCS}((T\leq T_c/2,\hbar\omega\leq\Delta/30)=$$

$$R^H_{res}(\omega,H)+r_0\omega^\beta\exp(-\Delta/kT)/kT; \qquad (1a)$$

This ansatz and the BCS theory for oxidized Nb fits excellently the T- and ω- dependencies of $R^H(T,\omega)$ of oxidized Nb cavities with averaged values r_0, β, and Δ/kT_c for a λ_{BCS}~100nm penetration layer changing with oxidation for RRR>100 Nb in characteristic ways [1-8]. By the weak interaction with phonons locally confined quasiparticles $|\epsilon|\leq\Delta_{ave}$ are easily driven out of thermal equilibrium yielding a saturating loss component named low field Q-slope (LFQ) [2b,5]

$$R_s(T,B>10 \text{ mT}) = a(T)/B^2 + R_{BCS}(T,\sim20mT) + R_{res} \qquad (1b)$$

whereas extended $|\epsilon|\geq\Delta_{ave}$ rf quasiparticles have long mean free path $l_{in}=v_F\tau_{in}(T,<10GHz)>6\cdot10^{-3}(T_c/T)^3$cm and so R_{BCS} does not heat its surface. At Nb_2O_5/Nb interfaces

via localized states $n_L\leq10^{21}$/cm^3 rf shielding current momenta are transferred to the lattice coherently
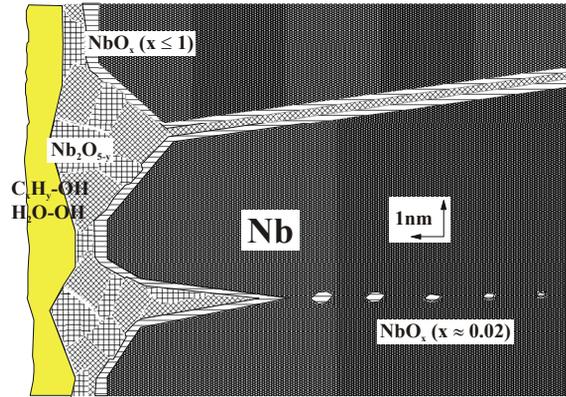
Figure 1: Nb surface with crack corrosion by wet oxidation by Nb_2O_5 volume expansion (factor 3). Nb_2O_{5-y}-NbO_x weak links/segregates (y,x<1) extend up to depths between 0.1– 1/1-100 µm for good/bad Nb quality and weak/strong oxidation [8-11]. The double layer $(OH)_yH_2O$ being chemisorbed by hydrogen bonds to NbO_x may be covered by $(C_xH_yOHOH_yH_2O \geq3nm)$ and dust.

$R^{PH}_{res}(T,\omega)= \{e\mu_0\omega\lambda_{BCS}(T)\min[l,\lambda_{BCS}(T)]n^2_L/v_F\}^2/\rho v_T$ (2a) with ρ as density, with v_T as transversal sound velocity and with l_s~3nm as surface mean free path of Nb causing *$R^{PH}_{res}\leq10^{-9}\Omega(f/GHz)^2$ by phonon generation. At Nb_2O_5 serrations in Fig.1 n_L cause weak links (WL) losses* $R^{WL}_{res}(T,\omega)\geq1n\Omega(f/GHz)^2$ (2b) being obvious in cold worked or thin film Nb cavities [4a,8]. Field dependent losses $R^H(T,H)$ can be written as Taylor series with the *first two terms named MFQ* $\delta R^B= R^1_{hys}(T,\omega)H/H_c + R^H(T_0,\omega,H)\gamma(T)(H/H_c)^2+$ (3a) by Josephson fluxons penetrating fast above H_{c1J} into WLs yielding the *fluxoid hysteric losses* $R^1_{hys}(T,\omega)$ $H/H_c=4/3\pi\omega|H-H_{c1J}|/2j_{cJ}(T)2\lambda(T)$ [2b,3,5,8]. As consequence R^{WL}_{res} and R_{hys} *heat the surface* enhancing γ

$R_{BCS}(T+\Delta T)=R^HH^2/2\{1+\gamma^*(T)(B/0.2T)^2+\cdots\}$ (3b) According to [5] HFQ is based on pair breaking caused by $E\cos\omega t$ with E>MV/m acting at localized states n_L in Nb_2O_5 with an energy gain 2zE>1meV above the energy gap $2\Delta^*$ being described quantitatively by $R^E(E)=b_sB^2/E^2s(-c/E,-c/E^0)\sim b^*(\exp(-c/E)-\exp(-c/E^0))$ (4) being dominated by crystallographic shear planes (CS) bordering crystallographic blocks (CB) with their low $\Phi_S=0.1eV$, i.e. $\kappa_S = 1.6$/nm, yielding $c_S = 2\kappa\Delta\epsilon_r/e\beta^* = 130 - 400$ MV/m by $\Delta \sim 1.5$ meV and by $\epsilon_{rS} = 20$ [5,10a]. In contrast to the qualitative model in [2b] the pair breaking $ezE\geq\Delta$ is treated in [5] yielding the *HFQ source term* $b_ss(E)$, feeding the *HFQ valve* and *HFQ-BCS loss terms* the latter defines Q_0. In Figs.2 Q_0 drops by more than a factor 10 without rf break down by l_{in}>mm of BCS

quasiparticles and $b_S(E)$ fits observation with a correlation factor $r^2 > 0.98$ [5].

NB OXIDATION

The improved understanding of Nb oxidation is based on older [10] and on recent surface science results [7,9,11] summarized below explaining differences between EP- and BCP- Nb removal [9c]. Tunnelling [12], ARXPS [10-11e], x-ray studies [11e,f], positron annihilation [11f] and $Z^H(T,H)$ [10] indicate gross differences between different $Nb_2O_5/NbO_x/Nb$ surfaces.

As **first step in oxidation**, O dissolves atomically in the open Nb lattice and migrates along grain boundaries and dislocations into the interior. Below about 500K as a **second oxidation** step the Cabrera Mott growth of Nb_2O_5 is based on the binding energy potential $V^O_m \approx 0.6V = b(O-O) - b(Nb-Nb)$ causing electrons n_C to tunnel through Nb_2O_5 charging O chemisorbed from lab air or vacuum. This yields electrochemical like Nb_2O_5 growth where V^O_m drives mainly (~80%) O ions through Nb_2O_5 toward the metallic $NbO_x(x \leq 1)$ surface to be discharged there and being injected into the Nb lattice or nucleate as CBs separated by CSs [10] needing a factor three larger volume straining the interface. At interfaces the surplus O and the Nb_2O_5 strain are relaxed in soft Nb by O injection and by creation of dislocations channelling O locally deep into Nb showing up, e.g. as crack corrosion in Fig.1. O precipitates under volume expansion in Nb as metallic Nb_6O or $NbO_x(x \leq 1)$ plaques or as dielectric Nb_2O_5 preferably at defects eased by ~100°C in LTB.

In *wet oxidation* the potential $V_m = V^O_m + V_d$ acts between the Nb/NbO_x metal and the charged NbO-OH-H_2O double layer with its dipole potential V_d. This waterous interface eases the O_2 ionisation and O^{2-} uptake into Nb_2O_5 where V_m results in fast transfer of O^{2-} along CSs via V_{OS} toward the NbO_x surface. In *BCP* a 4nm thick nano crystalline Nb_2O_5 grows repeatedly which by the volume increase above a factor 3 strain the Nb surface repeatedly and strongly. The localized strain is relaxed by local O injection and by dislocations creation yielding O transfer into larger depth <50µm. In *EP Nb is oxidized under potential control (~0.7V)* [11d] to Nb^{5+} ions dissolving in HF directly without strain by Nb_2O_5 crystallites. Hence in EP less dislocations are created transferring O into larger depth, i.e. most of the O surplus sticks at the surface. *Dry oxidation* of Nb with small dislocation densities, e.g. after annealing above 1000°C, is governed by an ordered, thin CB layer ($\leq$1nm) [11e] with $\Phi_B \sim 0.6eV$ [10a,12a,b]. Hence, the charging of chemisorbed O_2 and the transfer of O^{2-} are slow resulting in slow Nb_2O_5 growth ending at $d_O \sim 1-2nm$ and the reduced strain acting onto the interface reduces the dislocations creation, i.e. reduced O migration away from the surface. By defects dislocations or impurities CSs get nucleated as second layer and there V^O_m acts highly local.

The (UHV) baking at 120°C (LTB) eases relaxation of defects yielding a reduction of n_L in Nb_2O_5 [10a,b,11e] and of dislocations in Nb [7] and expansive precipitation

of Nb_2O_5, Nb_6O, and NbO_x out of the O lattice gas shifting H further into Nb [11i] with negligible O transfer from the oxide as measured by x-ray and SIMS [11f]. The LTB precipitation yields an NbO_x interface layer with 7.6 at% O in the first 10nm, i.e. reduced surface mean free path *l<2nm* [11e] instead of 3.6 at% O by room temperature air oxidation. By dissolution of the 2 – 4nm thick LTB oxide and afterwards wet oxidation (HF) about 2nm Nb with its precipitates are transferred to the wet oxide (~4nm) with less precipitates behind.

SUPERCONDICTIVITY OF OXIDZED NB

Clean superconducting (sc) Nb [10] shows $T_c = 9.25K$ and $\Delta_0/kT_c = 2.05$ degrading by O pick up, where 2at% O in solid solution degrades T_c and Δ by 20% and the mean free path *l* to <8nm whereas the d-bonded precipitates Nb_6O or $NbO_x(x \leq 1)$ act more strongly on *l* but less strongly on T_c and Δ as shown, e.g. by $\Delta \sim 0$ for disordered $NbO_x(x \sim 1)$. The d-bonded Nb_2O_5, Nb_6O or $NbO_x(x \sim 1)$ may precipitate out of atomically dissolved O at nuclei under volume expansion.

T*unnelling* through $Nb/NbO_x/Nb_2O_5/NbOOH/H_2O$ yields via leakage currents more then a factor 100 variations in $n_L(z)$ $\leq 10^{21}/cm^3$ with oxidation [12a,b], yields via I(U) normal conductivity for a *1.5nm thick surface layer* [12c] and the $T_c^* \sim 7K$ phase at interfaces [12d] confirmed by $Z(T,\omega < MHz)$ [9d]. Information on the *upper 100nm Nb* is given by $R_{BCS}(T,\omega,H)$ in its T, ω and H dependencies. For example, BCP wet oxidation yields for large grained Nb a Δ_{ave}/kT_c reduction down to 1.7 and for small grained or defective, e.g. cold worked Nb, down to ~1.8. The latter observation is explained by precipitation of O at nuclei. Those precipitates smear the energy gap by $\Delta^* \leq \Delta_{ave}$ plaques reducing $R_{BCS}(<15GHz)$ shown by $\beta(<15GHz) \sim 2$ in Eq.(1a) [4b] and enforcing LFQ in Eq.(1b) [4a]. The amount of O in the upper 100nm is in excess of 2at%, i.e. 20% gap reduction, as shown by $R_{BCS}(T, l<8nm)$ fits yielding $\Delta_{ave}/kT_c \geq 1.7$. As precipitate this amount relates: to the $T_c^* \sim 7K$ phase found by tunnelling [12d], by $Z(T \sim T_c^*, \omega < MHz, H_{dc})$ jumps [9a,d], by r_{32} increases [9b,c] or by the coherent onset ratio $H^{coh}_{c3}/H_{c3} \sim T_c^*/T_c$ in [9b,c]. By surface physics means 3.6 at% O by room temperature air oxidation grows by LTB to 7.6 at% O in total amount in the first 10nm [11e], the latter is related to precipitation without long distance diffusion in line with [11f] and with ordering reducing the density of n_L [5] or of dislocations [7]. In BCP the repeated straining by Nb_2O_5 crystallites is relaxed by repeated O injection and by repeated dislocations creation [7] channelling O away from the surface into larger depth, hence r_{32} increases by about 10%, only [2,5,9], *longer Nb_2O_5 filled weak links* (WL) are created enhancing R_{res}, R_{hys} and MFQ, pinning sites occur up to depths of 50µm found by low frequency impedance measurements in the super- conducting state [9]. As discussed above, in *EP the continuous injection of O into Nb* with only one final wet oxidation results in less

strain, i.e. less dislocations channelling O away form the surface, and so O sticks to surface resulting: in r_{32} increases by about 20%, in weakened HFQ, R_{res}, R_{hys} and MFQ and in reduced pinning up to depths of 10µm found [9c]. In both cases by *LTB O precipitates* at the surface: enhance
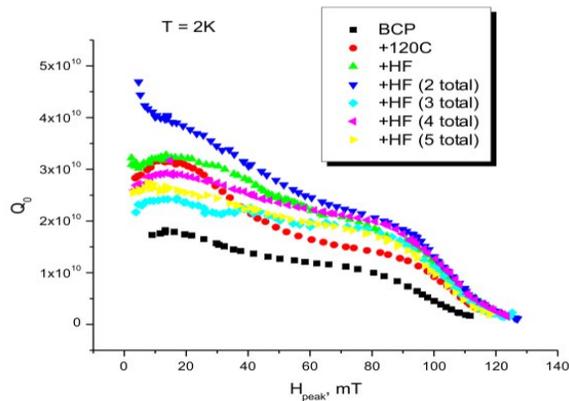
Fig.2a: Q(2K,1.3GHz,H) of fine grained, BCP stripped Nb, treated by LTB and several HF stripping.
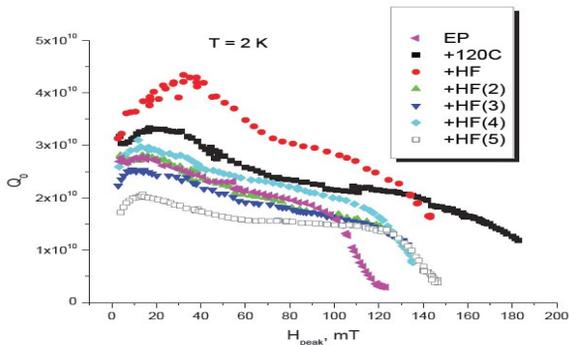
Fig. 2b: Q(2K,1.3GHz,H) of fine grained, EP stripped Nb, treated by LTB and several HF stripping.

R_{BCS}(4.2K,<15GHz), enhance Δ_{ave}/kT_c to 1.85-1.9 in Eq.(1a), enforce LFQ in Eq.(1b) [2b,5], reduce $l_S<2nm$, enhance r_{32} by about 10% [9], whereas b_S in Eq.(4) is is reduced by several orders of magnitude [5].

DISCUSSION

Above it has been clarified that the main differences between BCP- and EP- oxidative Nb removal is the repeated Nb_2O_5 crystallite (~4nm) growth in BCP, which causes repeated strain and O injection causing repeated dislocation creation channelling O away from the surface deep into Nb as shown: by WL growth enforcing R_{res}, R_{hys} and MFQ [1], by severe HFQ, by little r_{32} increases and by enforced pinning up to depth of about 50µm [9]. In the case of EP, fewer dislocations, i.e. fewer WLs, are created and O stays at the surface enhancing r_{32} and reducing HFQ and R_{res}, R_{hys} and MFQ. By LTB, O precipitation is enforced at the surface enlarging r_{32}, R_{res}, R_{hys} and MFQ but weaken HFQ [5]. Aside of defects created by oxidation, defects may be there from the beginning as in the case cold worked Nb [5] with enforced WL growth in

oxidation enhancing: R^{WL}_{res}, R^1_{hys} and MFQ showing up in ΔZ increases [9a,c].

Whereas it is well accepted that EP results in better Nb cavities then BCP shown clearly in [1], the surface physics behind those findings is modelled here for the first time. Whereas by BCP in Fig.2a R_{res} is only slightly enhanced over R_{res} of cold worked Nb [5[the HFQ onset is shifted in this cleaner and smoother Nb to much higher fields but still EP data in Fig.2b show further improvement of R_{res}, R_{hys}, MFQ and HFQ. By LTB R_{res}, R_{hys}, MFQ weaken, LFQ strengthens and HFQ improves especially for EP surfaces. By HF stripping of the dielectric LTB oxide coating and wet oxidation afterwards the O precipitate rich region is replaced by cleaner Nb [11e] therewith LFQ is reduced and R_{res}, R_{hys} and MFQ improve hinting to the fact that those locally confined quasiparticles $|\epsilon|\leq\Delta_{ave}$ and WLs grow in density toward the LTB surface in line with the O concentration in [11e]. With further HF stripping HFQ reappears where Q_0 is defined by HFQ BCS loss term with its long mean free path not heating the surface, i.e .not causing thermal runaway.

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