Nitrogen doping and the performance of superconducting radio-frequency niobium cavities: insights from neutron diffraction and neutron Compton scattering

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Abstract. Neutron Compton scattering and neutron diffraction have been applied to investigate the influence of nitrogen doping of niobium on the performance of superconducting radio-frequency niobium cavities. To this end, a comparative study of the neutronic response of two samples has been performed. An electro-polished and nitrogen-doped niobium sample was compared with a standard, a niobium sample that has only undergone the electro-polishing procedure. The first piece of information, provided by neutron diffraction, is that additional conditioning of the electro-polished cavity material, through doping with nitrogen, leads to a systematically larger niobium lattice expansion, which provides an upper conservative limit of nitrogen concentration consistent with values reported in the literature. Furthermore, neutron Compton scattering shows a broadening of the niobium momentum distribution in the nitrogen-doped sample, as compared to the standard, thus indicating an increased degree of ordering and binding of niobium in the metal lattice. On the whole, these observations suggest that nitrogen-doping leads to some degree of lattice ordering, most likely due to increased hydrogen trapping, in agreement with previous results using surface spectroscopy.
1. Introduction

Modern particle accelerators greatly rely on state-of-the-art superconducting low-dissipation niobium (Nb) radio-frequency cavities (SRFCs). Understanding the structure-performance relation of SRFCs is thus of crucial importance. One of the most important findings in this respect has been that SRFC performance is compromised by the presence of hydrogen (H) near the cavity surface [1,2]. Depending on the level of H concentration, two scenarios of the quality-factor (Q) degradation are known: (i) H Q-disease which degrades cavity performance even at low accelerating gradients; and (ii) High-Field Q-slope (HFQS) which is caused by the strong increase in residual resistance at high accelerating fields. H can be present in SRFCs both as an interstitial in the Nb lattice and in the form of non-superconducting $\epsilon$ and $\beta$ Nb hydride phases, as evidenced by Scanning Electron Nano-area Diffraction (SEND) [2]. It has been shown that several micrometer-sized Nb hydride inclusions, which are not superconducting and form in Nb near the SRFC surface upon cavity cool down, are responsible for Q-disease [1].

Several mitigation strategies for Q-factor degradation in SCRFs have been identified so far. Temperature-dependent TEM studies have demonstrated precipitation of Nb nanohydrides within the penetration depth at cryogenic temperatures in HFQS-limited electropolished (EP) cavities [2]. 800 °C bake of Nb cavities was empirically found to eliminate Q-disease and HFQS-free cavities which underwent 120 °C bake showed significantly reduced hydride formation [1,2]. A reduction of Nb-hydride precipitation appears to be caused by the introduction of stable H-vacancy complexes during 120 °C bake [3,4]. Recently, the Linac Coherent Light Source-II Project at Stanford accepted a novel nitrogen doping (N-doping) technology [5] for the production of 280 cavities. Discovered at Fermilab, N-doping systematically improves Q up to a factor of three [2]. A combination of annealing in a partial pressure of $N_2$ gas and subsequent EP of the Nb cavities leads to several hundred ppm of N on the Nb surface. Being extremely efficient at medium fields, N-doped cavities are limited by the quench at high accelerating fields.

Current research efforts by the SRFC community are concentrated on finding the origin of the limitation of the N-doped cavity quench, seeking to understand how N-doping and Nb sample baking cause an increase in performance. In an attempt to address these efforts, this work reports on investigations of nitrogen-doping-induced changes to structure and dynamics of conditioned niobium samples mimicking SRFC cavities. In this work, we have extended the traditional SCRFC research programme, chiefly consisting of surface probes, by employing a combination of neutron Compton scattering (NCS) and neutron diffraction (ND).

The advocated approach seems very timely, as electron and X-ray diffraction-based methodologies have already been successfully applied in the characterisation of SCRFs [2] and ND is a natural extension of this line of research. NCS can also be a source of valuable information about the nuclear dynamics that can be linked to local material properties, especially at the interface between ordered and disordered environments [19,23,24]. In this latter context, NCS provides a unique capability as it can be used to measure nuclear kinetic energies and other nuclear quantum effects (NQEs) in a mass-resolved manner [19,23,24]. Moreover, NCS can in principle access NQEs at any temperature, in a manner unaffected by the Debye-Waller factor [19,23,24]. NCS can also be used in a wide variety of samples and sample environments, with samples of different shapes, sizes, densities, textures and transparencies to radiation, thus beating other neutron-based materials characterisation techniques like reflectometry or small-angle neutron scattering, where sample thickness and surface roughness may render experiments unfeasible [24].

The proposition to employ NCS as a new technique for cavity material characterisation is also very timely in the light of recent modelling efforts reported in the SCRFs-related literature where Zero Point Energy (ZPE) effects have been shown as a very relevant ingredient, crucial for the understanding of the energetic, thermodynamic and electric properties of SCRFs [7]. More importantly, however, NCS together with ND continues to be relatively unexploited yet powerful
combination of techniques as applied on the VESUVIO+ spectrometer at the ISIS Facility in the UK [10, 11, 19, 22–24].

2. Methodology and Results

In what follows, the methodology and results of NCS and ND experiments on two Nb samples mimicking two different types of Nb SCRFs will be described. To this end, two Nb samples, representing two different cavity-material treatment protocols, were prepared from the same Nb sheets that cavities are made out of and investigated at temperatures of 80 K and 300 K. The samples were prepared using the same chemical processes and the same furnaces that are used for the actual cavities: an EP sample (hereinafter denoted as Nb1) and a sample that has been subjected to N-doping (hereinafter denoted as Nb4).

In essence, an NCS spectrum measured by a particular detector (at a given scattering angle \( \theta \)) and at a given time-of-flight (TOF) value, \( t \), is a sum of neutron Compton recoil peaks centred at mass-dependent TOF values, (see Fig. 1, lower inset). Mathematically [10,12,14–16,18,19,23,24],

\[
C(\theta, t) = A \frac{E_0 I[E_0]}{q} \left[ \sum_{M} c_M J_M(x_M) \otimes R_M(x_M) \right],
\]

where, \( M \) is the mass of a given nuclide, \( (M = Al, Nb) \), \( A \) is a proportionality constant, \( E_0 \) and \( I[E_0] \) are the incident neutron energy and intensity, respectively, and \( q \) the neutron momentum transfer to the sample. Moreover, \( J_M(x_M) \) is the unit-area-normalised longitudinal momentum distribution (NMD) of a nucleus of mass \( M \), \( R_M(x_M) \) is the mass-dependent resolution function, the symbol, \( \otimes \), implies the convolution product between the aforementioned functions, and \( c_M \) are coefficients proportional to the product of the number density and the total bound neutron cross section of a given nuclide [19]. The experimental curve for an isolated recoil peak for a given mass \( M \) (see Fig. 1, main), expressed in the harmonic and isotropic lattice limit (HL) is of the form \( J_M(x_M) \otimes R_M(x_M) \) with

\[
J_M(x_M) = \frac{\exp(-x_M^2)}{\sqrt{2\pi\sigma_M^2}} \left[ 1 - \frac{\sqrt{2} \sigma_M}{q} H_3(x_M) \right]
\]

where \( x_M = (y_M)/(\sigma_M\sqrt{2}) \), \( y_M \) is the longitudinal nuclear momentum for a given nuclide of mass \( M \), and \( \sigma_M \) is the standard deviation of \( J_M(x_M) \) [19,23,24]. The second term in Eq. (2) accounts for deviations from the IA, also known as final states effects (FSEs), expressed here in the HL limit [14,16].

In this work, NCS data were measured at a total of 132 detectors over the angular range of 130 to 170 degrees using a double-difference configuration offering improved resolution in back scattering [8,19]. The samples were loaded into aluminium (Al) containers of 0.1 mm wall thickness and placed inside a dedicated closed-cycle helium refrigerator. Each sample was a plain Nb slab of cross-sectional area 2x3 cm\(^2\) and 3 mm thickness. Sample Nb1 was prepared to contain no traces of nitrogen (N). Sample Nb4, subject to N doping, was expected to contain sub-percent N concentrations.

The NCS data reduction and fitting was performed according to standard procedures, detailed elsewhere [10,12,14–16,18,23,24]. The procedure applied to raw TOF spectra, recorded by each backscattering detector, consisted of a pre-fit of the raw data, the calculation of sample and container-dependent multiple scattering (MS) signal, the subtraction of the MS signal and the MS-corrected container signal, the subsequent focusing of corrected data into the longitudinal momentum space of Nb, and finally the fit of the focused data to obtain the longitudinal Nb momentum distribution curves, from which the values of the standard deviations of Nb longitudinal NMDs were extracted.
Focused and normalised-to-unit-area NMDs of Nb1 and Nb4, recorded at 80 K, are shown in Fig. 1. It can be clearly seen that both the maximum value and the position of the maximum of the NMD is lower for Nb4 compared to Nb1. To guide the eye, an inset has been added and placed on the left hand side within the main figure. Green dashed lines and a green arrow indicate this trend. The observed shift of the NMD maximum, \( y_{\text{max}} \), towards lower (more negative) \( y_{\text{Nb}} \) values, given the mathematical form of the NMD in the HL limit (Eq. (2)), signifies an increase of the NMD standard deviations. A rough estimate, based on the position and the direction of the green arrow, gives a shift of \( y_{\text{max}} \) ca. -2.5 Å\(^{-1}\) between samples Nb1 and Nb4. It is in fact possible to estimate the standard deviation (STD) of an NMD within the harmonic lattice limit (HL) solely based on the position of the NMD peak maximum. To this end, another contribution to this volume series has been prepared [25]. In a nutshell, the method uses the fact that, within the HL and in the presence of FSEs, Eq. (2) can be differentiated with respect to the \( x_M \) variable to find the maximum of \( J_N(x_M) \). This maximum proves to be a function of \( \sigma_M \) which is a solution of a rather complicated multiply-nested radical equation [25]. However, in addition to the exact analytic solution one can obtain an approximate solution and use the fact that an FSE correction only slightly shifts the position that the NMD maximum would have otherwise had in the IA limit, \( y_{\text{max}} = 0 \). Thus, consequently \( y_{\text{max}}^2 \ll (\sigma^2_M + s^2_M) \), where \( s \) is the standard deviation of the mass-dependent instrument resolution function, \( R_M(x_M) \). One then can obtain an approximate solution to be refined through an iterative process with the zeroth iteration solution given by [25]:

\[
y_{\text{max}}^{(0)} = -\frac{\sigma^4}{q(\sigma^2_M + s^2_M)}
\]  
(3)

Equation (3) can be used to estimate the STD change of NMDs when going from sample Nb1 to Nb4. However, due to the fact that, as can be seen in Figure 1, the NMD of Nb1 has its maximum very close the the IA limit, i. e., \( y_{\text{max}} = 0 \), using Eq. (3) to estimate the NMD STD for the Nb1 sample would lead to a very unprecise estimation. Thus, a different strategy was adopted. Using the combined knowledge of the backscattering kinematics for \( M = 93 \) amu and the instrument resolution function \( R_M(x_M) \) characteristics published elsewhere (see, e. g. [23]) we obtain two important clues to this end. Firstly, the values of the momentum-transfer, \( q \) for the backscattering detectors under investigation vary only very slightly between 90 and 94 Å\(^{-1}\) and we can assume, for the sake of this estimation, an average value \( q = 92 \) Å\(^{-1}\). Secondly, the STD of the total instrument resolution function for \( M = 93 \) amu also does not vary markedly across the whole range of the backscattering detectors with an average of \( s = 29 \pm 1 \) Å\(^{-1}\). Furthermore, expecting a difference between NMD STDs of Nb1 and Nb4 to be very small, one can plug in \( \sigma + d\sigma \) into Equation (3) and then Taylor-expand treating \( d\sigma \) as a small expansion parameter while keeping \( q \) and \( s \) constant. This leads to the following expression:

\[
\Delta y_{\text{max}}^{(0)} = y_{\text{max}}^{(0)}(\sigma + d\sigma) - y_{\text{max}}^{(0)}(\sigma) \approx \frac{d\sigma}{q} \left( \frac{4\sigma^3}{2\sigma^2 + s^2} - \frac{2\sigma^5}{(s^2 + s^2)^2} \right)
\]  
(4)

Substituting \( q = 92 \) Å\(^{-1}\), \( s = 29 \) Å\(^{-1}\), and \( \Delta y_{\text{max}}^{(0)} = -2.5 \) Å\(^{-1}\) first into Equation (3) and then, using the obtained solution, to Equation (4), one obtains \( \sigma = 17 \) Å\(^{-1}\) and \( d\sigma = 7 \) Å\(^{-1}\) for the Nb4 sample. The obtained value of \( d\sigma \) shows the right trend visible in the NCS data. Its numerical value is, however, rather too high. This is a simple consequence of the fact that the method to estimate STD of an NMD from the NMD peak position maximum relies inherently on the sensitivity of the peak position to both \( q \) and \( \sigma \), a sensitivity which is the largest for smaller masses (e. g. protons).

Another robust method of the estimation of the STDs of NMDs come to mind in the context of the above calculation, the difference method [26]. In this method, the difference of two
NMDs is fitted with the differenced NMD shapes modelled either as simple Gaussian functions for harmonic and isotropic local potential, or and an analytical Gauss-Hermite expansion for an anharmonic or anisotropic potential. In case of Gaussian NMDs, whenever the difference $\delta$ between two NMDs, characterised by two different values of $\sigma$, $\sigma_2$ and $\sigma_1$, is small compared to their average, $\sigma$, the difference of NMDs can be expressed as a Taylor expansion in powers of $\delta/\sigma$ [26]. Unlike the method relying on FSEs and peak positions, described above, the NMD differencing method was demonstrated to work well for heavy masses, with copper and aluminium samples, measured at ambient and low temperatures, used as worked examples in the original work introducing the method [26]. Again here, a quick look on the difference between $J(y_{Nb4})$ and $J(y_{Nb1})$, shown as an inset on the right hand side of the main frame of Figure 1, shows that the quality of the difference signal is rather poor with the shoulders characterised by low signal-to-noise ratio and spurious spikes and other unresolved signals that would have not allowed for high precision estimation of the difference of NMD widths. However, similarly as in the case of the peak-maximum method described above, also here, the general trend can be inferred from the shape of the difference signal. This shape is characteristic for a difference between an NMD characterised by a larger width (here, sample Nb4) and the one with a narrower NMD (here, sample Nb1).

Encouraged by the qualitative insights yielded by both the NMD peak-maximum and the NMD-difference method, the fitting of focused Nb NMDs, recorded at $T=80$ K and $T=300$ K, was performed using Eq. (2). The fitting results confirm the qualitative insights pointing at systematic broadening of the NMD profile of the Nb4 sample, as compared to the Nb1 sample. The results of the fitting procedure, including the values of the STDs of NMDs for Nb1 and Nb4, are listed in Table 1.

Following the NCS analysis, we proceeded to analyze the ND data concurrently recorded using the high resolution ($\Delta \lambda/\lambda = 0.003$) backscattering VESUVIO+ detector bank [11]. The data were first normalised by point-wise division with Vanadium (V) data separately recorded.

Figure 1. Main: Focused and normalised-to-unit-area $J(y_{Nb})$ data, recorded for Nb1 (black trace) and Nb4 (red trace) at 80 K. Left inset: close-up around the $J(y_{Nb})$ maximum. Right inset: difference between $J(y_{Nb4})$ and $J(y_{Nb1})$. See text for details.
Table 1. Nb NMD widths together with 1-STD errors (in units of Å$^{-1}$). See text for details.

| Sample | T = 80 K | T = 300 K |
|--------|----------|-----------|
| Nb1    | 11.6 ± 0.1 | 18.2 ± 0.1 |
| Nb4    | 11.8 ± 0.1 | 18.5 ± 0.1 |

Figure 2. Nb4 ND data recorded on VESUVIO+ at 300 K. Black markers – ND data, red line – Le Bail-refinement of the data, blue line – residuals.

on the same instrument. Before division, V data were smoothed to exclude regions with Bragg peaks by fitting a fifth-order Chebyshev polynomial. Finally, Le Bail-refinement was performed using the JANA2006 program [27] with a background simulated by a fifth-order Chebyshev polynomial. An example of the result of this procedure is shown in Fig. 2 for the Nb4 sample at T=300 K. Figure 3 shows the ND data and fit for the Nb1 sample at T=300 K.

Table 2. Nb lattice constants together with 1-STD errors (in units of Å) from the Le Bail-refinement of the ND data recorded for samples Nb1 and Nb4 at T=80 K and T=300 K. See text for details.

| Sample | T = 80 K | T = 300 K |
|--------|----------|-----------|
| Nb1    | 3.2899 ± 0.0002 | 3.2954 ± 0.0001 |
| Nb4    | 3.2923 ± 0.0002 | 3.2978 ± 0.0002 |
The Le Bail fits, both at T=80 K and T=300 K (see Table 2) yield Nb4 lattice spacing values that are systematically, by ca. 0.002 Å (ca. 10 STDs) higher than the Nb1 lattice spacing values. This result, together with the result of the NCS analysis described above, constitutes, to the best of authors’ knowledge, the first demonstration of a rather unprecedented capability of Vesuvio+ to pick up very subtle structural and dynamical signatures of sample conditioning-induced local disorder for nuclei with such a high atomic mass (93 amu). In what follows, we will present a qualitative interpretation of this striking result.

3. Discussion

It is generally believed that the presence of adsorbed gasses in the Nb lattice leads to a systematic increase in lattice spacing. Diffuse X-ray scattering data of H trapping at N sites in the Nb lattice in the temperature range of 50–450 K by Metzger showed that, for a 1.1% N concentration, the lattice parameter change due to the presence of H, $\Delta a_H = a(NbN_{0.011}H_{0.008}) - a(NbN_{0.011})$, increases with increasing temperature, whereas the analogous figure for N, $\Delta a_N = a(NbN_{0.011}) - a(Nb)$, shows a less pronounced increase (see Fig. 5 in Ref. [28]). The values of $\Delta a_H$, inferred from this X-ray work, are ca. 0.0011 Å and ca. 0.0014 Å, at T=80 K and T=300 K respectively, whereas the values of $\Delta a_N$ are ca. 0.0045 Å and ca. 0.0047 Å. Moreover, Nb lattice constants have been shown to depend linearly on H and N concentration at T < 300 K [36,37]. Additionally, one can assume that: (i) at sub-percent H and N concentrations lattice expansion due to the uptake of N is independent on the expansion due to the uptake of H; (ii) both Nb1 and Nb4 contain the same amount of H due to the presence of the protective Nb$_2$O$_5$ surface layer which remains intact during sample conditioning; and (iii) Nb1 does not contain any traceable amounts of N. Based on these assumptions and on the values of the lattice constants listed in Table 2 one can obtain an upper conservative limit of the N
concentration in Nb4 of 0.0024/0.0045 · 0.011 ≃ 0.6 %, a value ca. 40% less than the value obtained by Metzger [28]. Considering the fact that the above limits obtained from ND are bulk values, this result is consistent with the maximum N concentrations measured using the SIMS technique over the first few microns of the surface of the N-doped Nb cavity samples (10^{20} N atoms per cm^3, corresponding to an average stoichiometry of NbN_{0.0018} [33]).

The ND results presented above are further corroborated by the NCS results by noting that Nb4 NMD widths are systematically and consistently (at both T=80 K and T=300 K) higher than Nb1 widths. In general, increased NMD widths measured in a crystalline sample signal a surplus of states in the atom-projected vibrational density of states (apVDOS) due to tighter binding of a given atom in the lattice [19, 23, 24] which may be the consequence of lattice ordering, e.g., when going from a glassy to a crystalline state [23, 24].

Using lattice theory when analysing X-ray diffuse scattering distribution in the Nb-H-N system, Dosch et al [31] showed that any H site which contributes more than 0.05 Å to the displacement of the two Nb neighbours of N in the direction of the crystallographic c-axis must be excluded from being a possible trap site for H. Only the nearest Nb neighbours of H experience a displacement of this order of magnitude [32]. Inelastic neutron scattering experiments in the Nb-N-H system show that the local mode energies of H in the untrapped and trapped states remain unchanged [30], thus leading to the conclusion that H remains in tetrahedral sites while being trapped at a remote enough position from the N atom to leave the local potential undisturbed.

Based on these observations, a model was built in which H atoms are placed so far apart from the N atoms so that no single Nb atom becomes a nearest neighbour for both of them [28]. In such a scenario, the dynamical coupling of Nb to H and N, the changes of the local potential felt by H, N, and Nb, and finally the changes in apVDOS are too small to manifest themselves markedly in Nb NMDs. Moreover, using the Dosch model [31] and the fact that the Debye temperature of Nb is constant in the temperature region 80–300 K [29], one can predict that untrapped protons present in the Nb lattice should systematically increase the displacement of the two Nb neighbours by at least 0.05 Å, on top of the temperature effect associated with the Boltzmann statistics of vibrational states. Using the pure-Nb Debye temperature of 284 K and assuming ca. 0.025 Å displacement surplus per Nb atom in the lattice, one obtains a decrease of the Nb NMD width of the order of 0.2 Å^{-1}. This prediction is in a very good agreement with the trend visible in Table 1: the Nb NMD width in Nb1, at both 80 K and 300 K, is lower by 0.2 Å^{-1} from the Nb NMD widths in Nb4. This observation signals lattice-induced NMD changes and seems to point towards an increased fraction of untrapped protons in Nb1, as compared to Nb4 in the temperature range 80–300 K.

On the whole, N doping and baking of the Nb in Nb4 seems to lead to some degree of Nb lattice ordering induced by increased H trapping (as compared to Nb1). This conclusion is in line with the result of Pfeiffer postulating H trapping by interstitial N atoms where only N-H pairs (and no higher agglomerates) are formed as the temperature is lowered [6]. However, two scenarios are still possible within this model. If the N concentration exceeds the H concentration in the Nb lattice, the variation of the temperature does nothing but to reversibly create and cleave N-H pairs in dynamics equilibrium [28]. In this scenario, for any choice of reasonable parameters, all the H atoms will be trapped below 120 K and the percentage of trapped H atoms decreases with increasing temperature with the final trap concentration at 300 K still amounting to about 40-60% [35]. Conversely, if the H concentration is higher than the N concentration, some H atoms might still not be trapped below 120 K and the final trap concentration may be much lower than 40% at room temperature. The presented analysis points towards the latter scenario.

4. Summary and Outlook
In summary, the analysis of ND and NCS results in electro-polished and N-doped Nb samples, prepared to exactly mimic two different types of state-of-the-art SRFCs, seems to be consistent
with previous electron microscopy results indicating the coexistence of nano or micro domains of at least two H-containing Nb phases embedded in the Nb lattice [1–4]. Moreover, the results presented here are in line with previous surface spectroscopic work suggesting that N is present as an interstitial in the Nb lattice, possibly binding or trapping H [2,6]. The NCS analysis presented in this work shows that N doping and baking of the Nb sample leads to some degree of Nb-lattice ordering induced by increased H trapping. Due to trapping, the H-induced SRF resistivity increase is reduced and the occurrence of precipitation is shifted to higher H concentrations thus greatly improving SRFC performance. However, the N concentration in the Nb lattice may still be insufficient to trap all H atoms below 120 K.

Further NCS and ND research should be carried out along two clearly visible lines of work. Firstly, more data should be acquired at cryogenic temperatures to shed more light on the N doping-induced changes in cavity performance at temperatures relevant of the operation of these devices. Secondly, more systematic studies need to be performed on various SRF cavity cut-outs in order to prune out sample-specific trends from those induced by material conditioning.

On the methodological front, further ab initio materials modelling-augmented studies are highly desired. To this end, single-crystal ND and NCS measurements would provide a clear cut assessment of the role played by anisotropy of material properties. Moreover, single-crystal ND would enable an appraisal of the thermal diffuse scattering and single-crystal NCS would open the possibility to assess the degree of NMD anisotropy.

Traditionally, NCS has been used as a local probe of nuclear dynamics in condensed matter systems and molecules [23]. Capitalising on more than three decades of evolution of NCS as a technique, this work demonstrates, for the first time, an attempt to extend the realm of NCS applicability to simple devices, superconducting radio-frequency cavities. Moreover, this work paves the way for more use of ND and NCS in future studies of the performance of technologically relevant devices. The synergies between ND and NCS cannot be more emphasized as in the case of their concurrent application to the same system on the same neutron beamline. Further research using this paradigm in mind should, in this particular case, lead to SRFC performance optimisation and the improvement of SRFC surface-processing technologies.

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