Origin of dielectric loss at the Nb/oxide interface: Evidence for atomic two-level systems

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While several experiments claim that two-level system (TLS) defects in amorphous oxides are responsible for energy relaxation in superconducting resonators and qubits, only a few are able to provide quantitative explanation of their data. Here several models of dielectric loss are considered to explain available experimental data. These cavities contain only a single lossy material in their interior, the niobium/niobium oxide interface, making them convenient testbeds for analysis of TLS parameters. It is shown that the noninteracting model does indeed yield the best fit to experimental data, provided that a one-species model with sharp modulus of electric dipole moment is assumed.

Energy losses from TLSs arise from the coupling between the TLS electric dipole moment and the electric field produced by the device. The conventional noninteracting theory predicts steady-state energy loss described by the loss tangent [12, 13]

\[ \tan(\delta_{\text{TLS}}) = \frac{\pi p^2 \rho \tanh\left(\frac{\hbar \Omega}{2k_B T}\right)}{3e \sqrt{1 + \left(\frac{E}{E_c}\right)^2}}, \]  

where \( p = |p| \) is the modulus of the electric dipole moment of the TLS, which is averaged over all possible directions leading to the factor of 3 in the denominator, and \( \epsilon \) is the dielectric constant for the material where the TLS is embedded. The quantity \( \rho \) is an energy-volume density (dimensions of (energy × volume)^{-1}) for TLSs with energy splitting equal to \( \hbar \Omega \), where \( \Omega \) is the resonance frequency of the cavity; \( E \) is the electric field at the location of the TLS, and \( E_c \) is the characteristic electric field for saturation.

Saturation happens when \( E \gg E_c \), the number of excited TLSs is maximized (equal to 50% of the total) so the amount of energy flowing from TLS to photons is equal to the energy flowing from photons to TLS, making the loss tangent equal to zero. It can be shown that

\[ E_c = \sqrt{\frac{3\hbar}{2p}} \frac{1}{\sqrt{T_1 T_2}}, \]  

where \( T_1 \) and \( T_2 \) are TLS energy relaxation and homogeneous broadening (coherence) times, respectively.

Therefore, measuring the loss tangent as a function of cavity electric field (or input power) provides information on TLS properties. Most authors find difficult to interpret their experiments in terms of Eq. (1). One common approach is to replace the denominator in Eq. (1) by \( [1 + (E/E_c)^2]^{\beta} \), and let \( \beta \) be a free fitting parameter [14]. The motivation for this choice appears to be the modelling of slower saturation with increasing electric fields when TLSs interact with each other, leading to \( \beta < 1/2 \). The interaction between TLSs transfers energy from resonant TLSs to nonresonant ones, competing against saturation. In spite of this motivation, we are not aware of microscopic theory for \( \beta < 1/2 \), so the introduction of \( \beta \) should be thought of as a phenomenological assumption.
The fits to experimental data in the literature claim \( \beta < 1/2 \), suggesting that TLS-TLS interactions are indeed important, as highlighted by stochastic fluctuations observed in qubit-TLS evolution [15]. For example, [16] shows best fit \( \beta = 0.25 - 0.42 \) for 13 different samples of niobium, while [14] obtained \( \beta = 0.15 \) at different temperatures, and Fig. 9(e,f) of [17] shows a wide distribution of \( 0 < \beta \leq 1/2 \) for identical Nb samples as a function of oxide regrowth.

However, there was no attempt to fit statistical distributions for \( p \) and \( E_c \) (multiple species of TLSs) to the data as is commonly assumed in theories of amorphous materials.

The large spread in observed values of \( \beta \) for similar niobium samples raises the question: Could the non-interacting TLS model (with \( \beta = 1/2 \)) provide the best description under the additional assumption that other TLS parameters such as \( p \) and \( E_c \) are statistically distributed in amorphous materials? Such a distribution would also slow down saturation, in the same way that \( \beta < 1/2 \) does.

Answering this question may also shed light on the microscopic structure of TLSs causing loss. There are two known types of TLSs [18]: “Atomic TLSs” occur when impurities tunnel between pairs of equivalent sites. A notable example is Nb\( _x \)O\( _y \)H [19], where interstitial \( O \) creates a bistable trap for \( H \). Only two locations for \( H \) are stable for a given interstitial \( O \), leading to octahedral averaging of \( p \), with sharply defined \( p \). The other type is the “glassy TLS” realized by bistable configurations involving several atoms in an amorphous lattice [20, 21]. The wide variation in glassy TLS morphology indicates a broad distribution for \( p \), with implications for dielectric loss [22].

Here the question of whether a broad distribution of \( p \) is required to explain dielectric loss is investigated by proposing alternative data analysis of experimental data for TLS saturation. The focus is on the experimental data of Romanenko and Schuster [16], who measured quality factor \( Q \) in three-dimensional TESLA cavities made of high quality niobium (in contrast to the artificially doped samples of [19]). TESLA cavities made of Nb are known to achieve record-high resonance quality factors \( Q > 10^{11} \), and as a result variations of accelerating cavities adapted to quantum information processing are now under consideration [23].

TESLA cavities [24] have remarkable structural/materials simplicity when compared to the two-dimensional superconducting devices used in quantum hardware [25]. For example, they contain only one lossy material, the Nb/Oxide interface. As shown below, the absence of several lossy regions/materials simplifies data analysis, enabling the testing of more sophisticated models that take into account variations of \( p, E_c \) and the suitability of the parameter \( \beta \).

The Nb/Oxide interface can be made mostly of amorphous Nb\( _x \)O\( _y \), or crystalline niobium pentoxide Nb\( _2 \)O\( _5 \), depending on the type of surface treatment [17, 26–28].

![Cross-section of the electric field amplitude distribution for the TESLA cavity’s 1.3 GHz TM\( _{010} \) mode, normalized to \( W_{\text{total}} = 1 \) J of stored energy. The electric fields are axially symmetric about the z-axis.](image)

It was shown previously that TLSs are present in both types of oxide [17].

## II. Numerical Modelling of Dielectric Loss at the Surface of a Cavity

The resonance quality factor \( Q \) measured in experiments is given by \( 1/Q = \sum_i \tan(\delta_i) \times f_i \), where \( \tan(\delta_i) \) is the loss tangent for a certain region \( i \) of the device, and \( f_i \) is the corresponding participation ratio [6]. Participation ratio \( f_i \leq 1 \) is defined as the fraction of electric energy stored in the dielectric volume \( i \), normalized by the total electric energy in the device.

For the TLS mechanism, the loss tangent (1) depends on the value of the electric field at a particular point \( r \) in the device. Finite element software COMSOL was used to predict the electric field distribution of the 1.3 GHz TM\( _{010} \) mode for the TESLA cavity used in [16]. The results are shown in Fig. 1, where it becomes evident that the value of electric field varies by several orders of magnitude at the internal surface of the cavity, ranging from zero at the top of the elliptical cell to \( \approx 2E_{\text{acc}} \) at its edge. The “accelerator field” \( E_{\text{acc}} \) is defined as the accelerating voltage divided by the active cavity length [24].

As a result of this wide variation of electric fields it is crucial to express \( 1/Q \) as an integral over the surface \( S \) of the cavity,

\[
\frac{1}{Q} = \frac{1}{W_{\text{total}}} \sum_j c_j \int_S \frac{|\vec{E}(r)|^2}{\sqrt{1 + \frac{|\vec{E}(r)|^2}{\epsilon_{\text{eff}}^2}}} d^2r + \frac{1}{Q_{\text{non-TLS}}}. \tag{3}
\]

Here \( W_{\text{total}} \) is the total electric energy inside the cavity,

\[
W_{\text{total}} = \frac{1}{4} \int_V \epsilon(r) |\vec{E}(r)|^2 d^3r, \tag{4}
\]
and \( c_j \) models the loss tangent (1) arising from one particular “j” species of TLS. This is given by
\[
c_j = \frac{\pi}{12} p_j^2 \tanh \left( \frac{\hbar \Omega}{2 k_B T} \right) \rho_j',
\]
where \( p_j \) is its electric dipole moment and \( \rho_j' \) is its energy-area density (dimensions of (energy \times area)^{-1}). The quantity \( 1/Q_{\text{non-TLS}} \) models energy dissipation due to other mechanisms that do not saturate such as residual normal-state resistance due to thermal quasiparticles [29], piezoelectric effect [10], etc.

### III. FITTING EXPERIMENTAL DATA

Experimental data [16] for \( Q \) as a function of \( E_{\text{acc}} \) at \( T = 1.5 \) K for two different TESLA cavities is considered: (1) Electropolished cavity which was treated to remove most of the oxide layer on top of Nb, leading to a thin layer of mostly amorphous NbO\(_x\) estimated to be 5 nm thick; (2) Anodized cavity which contained a thick oxide layer made mostly of crystalline Nb\(_2\)O\(_5\), with thickness estimated to be 100 nm.

The \( Q \) vs. \( E_{\text{acc}} \) experimental data points were extracted [30] from Fig. 2 (electropolished) and Fig. 4 (anodized) of [16]. Only data points from the lowest \( E_{\text{acc}} \) up to just before the zero derivative point around \( E_{\text{acc}} \sim 5 \) MV/m are included in our analysis, because for larger \( E_{\text{acc}} \) the \( Q \) starts decreasing with increasing \( E_{\text{acc}} \), signaling that an additional mechanism of loss takes over.

The values of electric field at the surface of the cavity obtained by COMSOL for different \( E_{\text{acc}} \) were then used in conjunction with our Eq. (3) to obtain best fits as a function of fitting parameters \( c_j, E_c, \) and \( Q_{\text{non-TLS}} \). The oxide dielectric constant was assumed to be \( \epsilon = 33 \epsilon_0 \) but this choice did not affect the fittings due to the small volume of the oxide. The results are shown in Fig. 2a (electropolished) and Fig. 2b (anodized).

Various distributions and number of species were fit to the two experimental data curves using a nonlinear \( \chi^2 \) minimization algorithm. Uncertainty for the experimental error in measurements of \( Q \) were estimated to be lower than 10\% in [16], but in our view this estimate encapsulates both the statistical and systematic uncertainties. Consequently, this value greatly overestimates the uncertainty required for the \( \chi^2 \) calculation.

In order to calculate values of \( \chi^2 \) that properly represent fit quality and are able to detect overfitting we took the statistical error in the usual \( \chi^2 \) formula by taking the standard deviation of the \( Q \) fluctuations in the low \( E_{\text{acc}} \) plateau region, where \( Q \) is found to be independent of \( E_{\text{acc}} \). This allowed for the statistical error used in the \( \chi^2 \) calculation to be estimated. The 1\sigma errors for fitting parameters where found by manually adjusting one of the fitting parameters while holding the others constant until the value of \( \chi^2/\text{DoF} \) increased by 1 (DoF is the number of degrees of freedom, equal to the number of data points minus the number of fitting parameters).

The best fit for the electropolished cavity (5 nm thin oxide) was a one species plus non-TLS offset. As seen in Table I, this “one-species” fit led to a \( \chi^2/\text{DoF} = 1.03 \) quite close to 1, indicating an optimal fit within experimental uncertainty. In contrast, the “two-species” fit applied to this cavity led to \( \chi^2/\text{DoF} = 0.78 < 1 \), indicating “overfitting”.

We also included the fitting proposed in [16] that was based on the expression
\[
\frac{1}{Q} = \frac{F \delta_{\text{TLS}}(T)}{1 + \left( \frac{E_{\text{acc}}}{E_c} \right)^2} + \frac{1}{Q_{\text{non-TLS}}},
\]
which lumped the electric field distribution inside the cavity into a single participation ratio \( F \) for the oxide layer, and assumed the phenomenological exponent \( \beta \) to be a free fitting parameter. For the electropolished cavity this leads to \( \chi^2/\text{DoF} = 1.74 \) and \( \beta = 0.38 \), indicating a worse fit than our proposed one species model.

In contrast, the best fit for the anodized cavity (100 nm thick oxide) was instead a two species plus non-TLS offset. As seen in Table I the two-species fit led to a \( \chi^2/\text{DoF} = 1.05 \). In comparison, the one-species fit and a fit to Eq. (6) led to \( \chi^2/\text{DoF} = 4.40 \) and 2.72, respectively, both significantly worse than the two-species fit.

### IV. CONCLUSIONS

In summary, numerical modelling of TLS photon loss was applied to experimental data in TESLA cavities, providing some clues on the nature of the TLS defects that are present in the niobium/niobium oxide interface of superconducting devices. In contrast to previous analysis of the data [16], the noninteracting model for TLS dielectric loss [12] with \( \beta \) fixed at 1/2 was shown to lead to the best fit, provided that a one-species model is assumed in the case of an electropolished cavity with a thin oxide layer. This result contrasted with the case of an anodized cavity with thick oxide, where instead a two-species non-interacting model (also \( \beta = 1/2 \)) was required to provide the best fit.

Whether or not the interaction between TLSs can be described by a phenomenological parameter \( \beta < 1/2 \) is debatable. The results of Table I suggest that accounting for the distribution of \( p \) and \( E_c \) is at least as important as allowing \( \beta \) to vary from 1/2.

To test whether continuous distributions of \( c \) and \( E_c \) can provide an even better fit for the data, additional models with Gaussian and exponential distributions of parameters \( c \) and \( E_c \) were also considered as shown in Table II. These models did not provide better fits, supporting the conclusion that TLSs at the niobium/niobium oxide interface have a narrow distribution of \( c \) and \( E_c \), suggesting small variation in \( p \) and \( T_1T_2 \) for the TLSs, and thus small variation in microscopic structure.

The thin 5 nm oxide is mostly amorphous NbO\(_x\), with a small quantity of encrusted clusters of crystalline...
FIG. 2. Quality factor $Q$ as a function of $E_{\text{acc}}$ for the TM$_{010}$ mode of the TESLA cavity. The TLS model fit used in Ref. [16] (Eq. (6)) is shown as well. (a) Electropolished cavity, with 5 nm thin oxide. Here the one species plus non-TLS offset model provided the best fit with $\chi^2/\text{DoF} = 1.03$. The two species plus non-TLS offset model led to $\chi^2/\text{DoF} = 0.78 < 1$, indicating overfitting. (b) Anodized cavity, with 100 nm thick oxide. Here the two species plus non-TLS offset model yielded the best fit with $\chi^2/\text{DoF} = 1.05$. The fit for one species plus non-TLS offset led to with $\chi^2/\text{DoF} = 4.40$.

In contrast, the thick oxide of the anodized cavity can be thought to be composed of a thin amorphous “transition” layer made of NbO$_x$, followed by a thick crystalline Nb$_2$O$_5$ layer [17, 26]. Table I shows that its “species 1” parameter $E_{c1}$ is within 2$\sigma$ of the thin oxide’s $E_c$, suggesting that both share the same microscopic structure. In particular, this indicates that species 1 is located at the amorphous transition layer separating metallic Nb from the crystalline Nb$_2$O$_5$ in the thick oxide. However, parameter $c_1$ is larger than $c$ by 3.6$\sigma$, suggesting that the density of species 1 is larger at the amorphous transition layer of the thick oxide.

The best fit for the electropolished cavity implies the $E, T \to 0$ limit for the loss tangent in NbO$_x$, is $\tan(\delta_{\text{TLS}}) = 4c \times 2k_B \times 1.5K/(e \times 5 \text{ nm} \times h \times 1.3 \text{ GHz}) = 7.7 \times 10^{-4}$. This value is 13$x$ smaller than the estimate that neglected the electric field distribution [16], and is 4$x$ smaller than the typical loss tangent measured in quantum computing devices [6, 31]. The reduced tan$(\delta_{\text{TLS}})$ for TESLA cavities demonstrates the high quality of its oxide.

The sharp distributions of TLS parameters indicates the two species are atomic TLSs. It can be checked whether the best fits for $c_j$ and $E_{cj}$ are consistent with the Nb:O:H complex. To do this, consider that this TLS consists of an H atom tunnelling between the two equivalent “c” sites of Fig. 4 of [32]. This implies its $p = |e|d/2$, where $|e|$ is the proton’s charge and $d = \sqrt{2a/4} = 1.17$ Å, with $a = 3.30$ Å the lattice parameter for Nb. Assume $\rho' = \sigma/(\pi\Delta)$, where $\Delta/k_B \approx 3$ K is the spread in TLS asymmetry due to O strain [18], and $\sigma$ is the area density for Nb:O:H. Our best fit for the electropolished cavity then implies $\sigma = 1.6 \times 10^{15}/m^2$, or $1.8 \times 10^{-4}$ TLS per Nb atom at the interface, and $\sqrt{T_1T_2} = 45$ ps. These values are physical, suggesting that Nb:O:H is indeed a likely candidate.

The relevance of Nb:O:H is not yet emphasized in the quantum device literature [4, 5]. It highlights the importance of surface preparation methods that reduce oxygen interstitials [27], as well as hydrogen. Interestingly, hydrogen atoms adsorbed at the surface were also identified as a source of dielectric loss [33, 34] and magnetic (flux) noise [35, 36] in aluminum oxide.

Superconducting qubits and resonators are limited by energy loss due to TLS defects in the amorphous oxides that encase them. In order to devise surface/interface passivation methods that reduce this effect, the TLS microscopic structure must be better understood. Here several models with different TLS parameter distributions were contrasted to available experimental data.
This led to the conclusion that TLSs in high-quality niobium/niobium oxide are best described by a sharp distribution of TLS parameters. The same species of TLS appears to be present in devices with thin and thick oxide layers, suggesting that this “species 1” is characteristic of amorphous NbOx. In contrast, an additional “species 2” is required to explain defects at the thick crystalline niobium pentoxide Nb2O5. The small variation in TLS microscopic structure is indicative of “atomic TLSs” such as Nb:O,H, realized by an atom (H) trapped in one of two locations near an O interstitial.

| Model                      | Two Species Plus Non-TLS Offset | One Species Plus Non-TLS Offset | Romanenko et al. (2017) Fit | Anodized Cavity (100 nm Oxide) |
|----------------------------|---------------------------------|---------------------------------|-----------------------------|-------------------------------|
|                            |                                  |                                 |                             |                               |
|                            | E_c1 = (3.20 ± 0.28) × 10^7 V/m | E_c2 = (2.65 ± 0.61) × 10^7 V/m | E_c = (1.90 ± 0.17) × 10^7 V/m | E_c = (5.44 ± 1.29) × 10^7 V/m |
|                            | c1 = (5.52 ± 0.26) × 10^{-24} C^2/J | c2 = (4.95 ± 1.65) × 10^{-23} C^2/J | F_TLS = (2.40 ± 0.12) × 10^{-11} | E_c = (5.44 ± 1.29) × 10^7 V/m |
|                            | Q_{TLS} = (1.22 ± 0.03) × 10^{-11} |                               |                               | E_c = (5.44 ± 1.29) × 10^7 V/m |
|                            |                                  |                                 |                               | E_c = (5.44 ± 1.29) × 10^7 V/m |
|                            | E_c1 = (2.97 ± 0.27) × 10^7 V/m | c = (5.83 ± 0.26) × 10^{-24} C^2/J | F_TLS = (2.40 ± 0.12) × 10^{-11} | F_TLS = (2.40 ± 0.12) × 10^{-11} |
|                            | Q_{TLS} = (1.23 ± 0.03) × 10^{-11} |                               |                               | F_TLS = (2.40 ± 0.12) × 10^{-11} |
|                            | E_c1 = (2.97 ± 0.27) × 10^7 V/m | c = (5.83 ± 0.26) × 10^{-24} C^2/J | F_TLS = (2.40 ± 0.12) × 10^{-11} | F_TLS = (2.40 ± 0.12) × 10^{-11} |
|                            | Q_{TLS} = (1.23 ± 0.03) × 10^{-11} |                               |                               | F_TLS = (2.40 ± 0.12) × 10^{-11} |
|                            | E_c1 = (2.97 ± 0.27) × 10^7 V/m | c = (5.83 ± 0.26) × 10^{-24} C^2/J | F_TLS = (2.40 ± 0.12) × 10^{-11} | F_TLS = (2.40 ± 0.12) × 10^{-11} |
|                            | Q_{TLS} = (1.23 ± 0.03) × 10^{-11} |                               |                               | F_TLS = (2.40 ± 0.12) × 10^{-11} |
|                            | E_c1 = (2.97 ± 0.27) × 10^7 V/m | c = (5.83 ± 0.26) × 10^{-24} C^2/J | F_TLS = (2.40 ± 0.12) × 10^{-11} | F_TLS = (2.40 ± 0.12) × 10^{-11} |
|                            | Q_{TLS} = (1.23 ± 0.03) × 10^{-11} |                               |                               | F_TLS = (2.40 ± 0.12) × 10^{-11} |
|                            | E_c1 = (2.97 ± 0.27) × 10^7 V/m | c = (5.83 ± 0.26) × 10^{-24} C^2/J | F_TLS = (2.40 ± 0.12) × 10^{-11} | F_TLS = (2.40 ± 0.12) × 10^{-11} |
|                            | Q_{TLS} = (1.23 ± 0.03) × 10^{-11} |                               |                               | F_TLS = (2.40 ± 0.12) × 10^{-11} |

TABLE I. Summary of one and two-species best fits with model fits from [16] also shown for comparison.

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