On the Homogeneity of TiN Kinetic Inductance Detectors Produced through Atomic Layer Deposition

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The non-homogeneity in the critical temperature $T_c$ of an Microwave Kinetic Inductance Detector (MKID) could be caused by non-uniformity in the deposition process of the thin superconducting film. This produces low percent yield and frequency collision in the readout of the MKIDs. Here, we show the homogeneity that offers Atomic Layer Deposition (ALD). We report an improvement of up to a factor of 50 in the fractional variation of the $T_c$ for TiN MKIDs fabricated with Atomic Layer Deposition in comparison with MKIDs fabricated with sputtering. We measured the critical temperature of 48 resonators. We extracted the $T_c$ of the MKIDs by fitting the fractional resonance frequency to the complex conductivity of their resonators. We observed uniformity on the critical temperature for MKIDs belonging to the same fabrication process, with a maximum change in the $T_c$ of 60 mK for MKIDs fabricated on different wafers.

I. INTRODUCTION

MKIDs belongs to non-equilibrium superconducting devices, which principle of operation is based on the measurement of the electrodynamic response of the superconductor, by a change in the kinetic inductance when a photon is absorbed. The MKID has attractive features like high quantum efficiency, low theoretical noise limit, multiplex frequency domain, photon-number-resolving and energy resolving.

The MKID arrays designed for various instruments share many common structures. Usually, these structures include superconducting LC resonators (capacitor and inductor), transmission lines and antennas (See Figs. 2 and 3). The superconducting resonators (pixels) are the photon detectors, which active area consists of a meandered inductor that acts as the photosensor and an interdigitated capacitor (IDC).

The production process of an MKID consists of depositing a superconducting thin film on an insulating substrate and applying standard lithographic patterning techniques to produce a resonator structure. These simple single-layer structures permit the use of high-quality crystalline substrates and a wide variety of superconducting films, providing an opportunity to achieve extremely low dissipation, desirable for precision instruments.

One of the most important features of the MKIDs is their capability to multiplex into large arrays. This capability enables the MKIDs to be used as powerful new astrophysical instruments for ground and space arrays besides of an extensive variety of applications. For example, one of the first MKIDs built for a camera is found in the experiment ARCON[3]. In SuperSpec[4] it is used as a component of a spectograph, in the Olimp[5] experiment to study the Cosmic Microwave Background (CMB) and recently, the use of MKIDs has been growing as an element of readout for Qubits. In addition, the MKIDs have been proposed as WIMP dark matter detectors[10] and as devices for measuring the neutrino mass[11].

In spite of the advantage that the MKIDs provides to readout thousand of resonators coupled to one transmission line, in some cases, the MKIDs present problems such as non-uniformity, instability, low percent yield and frequency collisions between their resonators. These problems are usually believed to be associated with the process of deposition[11].

In this sense, we are investigating ways to increase the homogeneity in the deposition to improve the per pixel performance of our devices through new superconducting material systems and fabrication techniques. The route that we are currently exploring attempts to create more uniform films through the use of Atomic Layer Deposition rather than the more traditional sputtering method. ALD is a thin-film technique based on the sequential use of a gas phase chemical process. Some of the advantages that offer the use of ALD are the thickness and composition control[12]. The superconducting material selected is TiN, whose $T_c$ is usually below 6K[13]. The critical temperature of the TiN depends on the thickness[14] or the N$_2$ concentration[15]11[16]. Therefore, through the measurement of the critical temperature, we will assess the uniformity of ALD.

In this paper will discuss the uniformity of ALD by measuring the critical temperature of 48 resonators coming from four identical MKIDs. All the MKIDs were fabricated with deposition of TiN through Atomic Layer Deposition under the same conditions. The $T_c$ is extracted fitting the fractional resonance frequency change $\delta f_r(T)/f_r$ to some analytical expressions of the complex conductivity given by the Mattis-Bardeen theory. Finally, the reproducibility of the fabrication is investigated by measuring and comparing the resonance frequency $f_r$, loaded quality factor, $T_c$ and kinetic inductance $L_k$ of each resonator, where the variations are tried to explain through simulations of some fabrication processes.
II. SUPERCONDUCTING RESONATORS

In a.c. current, the Cooper pairs of a superconductor are accelerated storing energy in the form of kinetic energy. The energy is stored inside the superconductor a short distance \( \lambda \approx 50 \text{ nm} \) in the form of a magnetic field. This effect is added to the surface impedance \( Z_s = R_s + i\omega L_s \) of the superconducting material, where \( R_s \) describes a.c. losses at angular frequency \( \omega \) caused by electrons that are not in Cooper pairs and \( L_s \) is the surface inductance due to the reactive energy flow between the superconductor and the electromagnetic field\(^{15-19} \).

The \( L_s \) in a LRC resonant circuit is the inductive element, which is a function of the temperature-dependent kinetic inductance \( L_k^{20} \), which is inversely proportional to the critical temperature of the superconducting material \( T_c \).

The resonance frequency\(^{21} \) of the resonant circuit as a function of the kinetic inductance is given by

\[
 f_r(L_k) = \frac{1}{\sqrt{C_g(L_g + L_k)}},
\]

where \( C_g \) is the geometrical capacitance and \( L_g \) is the geometrical inductance.

The critical temperature of a resonator can be obtained by fitting the fractional resonance frequency change \( \delta f_r/f_r \) to the imaginary part of the complex conductivity of a superconductor\(^{22} \).

The fractional resonance frequency change can be expressed as

\[
 \delta f_r = \frac{f_r(T) - f_r(0)}{f_r(0)} = -\frac{1}{2} \delta \sigma_2(T) / \sigma_2(0),
\]

where \( \alpha \) is the ratio of the kinetic inductance and the total inductance of the resonator\(^{23} \) and \( \sigma_2(T) \) is the imaginary part of the complex conductivity, which has the following analytical approximate expression according to the Mattis-Bardeen theory\(^{21,22} \).

\[
 \frac{\sigma_2(T)}{\sigma_N} \approx \frac{\pi \Delta}{\hbar \omega} \left[ 1 - 2e^{-\frac{\Delta}{k_B T}} I_0 \left( \frac{\hbar \omega}{2 k_B T} \right) \right].
\]

Here \( \sigma_N \) is the normal conductivity, \( I_0(x) \) is the 0-th order modified Bessel function, \( \omega \) is the frequency of the a.c. and \( \Delta \) is the energy gap of the superconductor.

In TiN films it has been shown that the complex conductivity increasingly deviates from conventional Mattis-Bardeen theory due to a strongly disorder of TiN\(^{24} \). This phenomenon is observed in Fig. 10. However, the critical temperature of the superconductor is not affected by the disorder\(^{25} \) and we can consider that the \( T_c \) is fixed in all resonators. Therefore, we expect the same value of \( \delta f_r/f_r \) as a function of the temperature in all resonators.

We are using microwave techniques to obtain the resonance frequency \( f_r \) of each resonator. The complex transmission amplitude of a resonator \( S_{12} \) obtained from the network analyzer is fitted to the model of the total transmission\(^{26-28} \) of a notch type resonator coupled to the transmission line, given by

\[
 S_{12}(f) = ae^{-2\pi f f_r} \left( 1 - \frac{Q_i/Q_c e^{j\phi_0}}{1 + 2jQ_i \left( \frac{f_f}{f_r} \right)} \right).
\]
The right-hand side of Fig. 3 shows the details of the geometry of two resonators and the CPW. The separation with respect to the ground plane is identical for each pixel, $A = 102 \mu m$ and $B = 15 \mu m$ (see the labels in the figure). The CPW line is separated from the two ground planes by a distance $C = 60 \mu m$. The separation of the capacitors to the CPW line varies according to the expected strength of the coupling, reflecting on the value of $Q_l$. For the $Q_r$ resonators we have $D = 150 \mu m$, whereas for the low $Q_r$ ones we have $E = 18 \mu m$. The width of the feedline across the resonators is $F = 200 \mu m$, broadening to $G = 400 \mu m$ on the extremities, with a separation to the ground planes of $H = 120 \mu m$.

We simulated the 12 resonators previous to the fabrication to know their resonance frequencies, load quality factors, geometrical capacitance and geometrical inductance. The simulations of each of the 12 resonators are done separately in SONNET. Fig. 2 shows the geometry used for the simulation of one resonator. The input parameters for the 12 resonators were the same. The stackup from bottom to top, was 500 $\mu m$ silicon (Erel = 11.7) beneath 1000 $\mu m$ air (Erel = 1). The metallization on top of the silicon layer was TiN (surface resistance = 0, thickness = 0, and the kinetic inductance swept from 15 pH/sq to 40 pH/sq in steps of 2 pH/sq). There was a 50 $\Omega$ port on each end of the transmission line. From the simulation, we obtain the complex transmission amplitude $S_{12}$ (Figs. 8 and 9) and by doing a fit to equation (4), extracted the resonance frequency and loaded quality factor $Q_l$. Using $f_r$ and $L_k$, $L_g$ and $C_g$ were obtained by a fit to equation (1). The resonance frequency span of the 12 resonators ranged from 0.5 GHz to 4.5 GHz for kinetic inductance sweep from 15 pH/sq to 40 pH/sq. The loaded quality factors of the 12 resonators can be divided in two groups: six resonators with low $Q_l \approx 6 \times 10^3$ and six resonators with high $Q_l \approx 1.2 \times 10^5$.

IV. MEASUREMENTS

In Fig. 4 we show the transmission curves for the four MKIDs obtained at 103 mK and -40 dB. From top to bottom: A1 (blue), B1 (red), A2 (cyan), and B2 (yellow). The resonance frequencies are seen as sharp spikes in this plot. The oscillations and overall shape of the curve are due to the transmission line. The first 10 resonance frequencies are in the range 1–3 GHz and the other two from 4 GHz to 4.5 GHz. The spikes in the range from 3–4 GHz correspond to second modes of the resonance frequencies, as identified in the simulations.

Analyzing the resonance frequencies, from the four MKIDs A1, A2, B1, B2, we can identify the twelve resonance frequencies in the range 1-4.5 GHz (Fig. 4) similar to the simulation, where the MKID A2 contains the lower $f_r$ in all its resonators.
To verify the uniformity of ALD we proceed to extract the $T_c$ with the method proposed in Appendix B for all resonators. Fig. 5 shows a distribution of critical temperature of all resonators where we can see four distributions close to the expected critical temperature. The MKIDs from the first wafer correspond to the left-most distributions and the ones from the second wafer correspond to the right-most distributions. The critical temperature averages are 4.05 K, 4.05 K for B1, A1 and 4.11 K, 4.10 K for A2, B2, respectively.

Calculating the average differences in the critical temperature for the 4 MKIDs (taking as reference the MKID B1) and dividing between the maximum sigma error $\sigma_{T_c}$, we obtain values of $\Delta T_c / \max(\sigma_{T_{c1}}, \sigma_{T_{c2}})$ of 0.76 and 0.91 for A1-B1 and A2-B2, respectively.

To investigate if the value of $T_c$ is constant and independent of the function used to do the fit, we considered different functions\(^{29,30}\) to fit the $\delta f_r/f_r$ and obtained $T_c$. We found that the distribution of the critical temperatures shown in Fig. 3 is the same for all the proposed functions, just varying in the mean $T_c$, and the values of $\Delta T_c / \max(\sigma_{T_{c1}}, \sigma_{T_{c2}}) < 1$. This shows that the MKIDs from the same wafer have the same $T_c$.

The percent variations in the critical temperature achieved in sputtering for MKIDs of TiN\(^{31,32}\) are of the order of 25% and, in our case, the percent variation of A1-B1 and A2-B2 is 0.3% and 0.5% respectively. This shows that ALD leads to a better control in the critical temperature, even with MKIDs from different wafers, where the percent variation obtained is (1.9%).

Notwithstanding this low percent variation, it is obtained a high variation in the resonance frequency (Fig. 6) and a discrepancy in the loaded quality factor (Fig. 7).
The fractional change of the resonance frequency \( \delta f_r/f_{r,A2} \) (comparing the resonators 1,...,12 from the MKID A2 with the resonators 1,...,12 from the MKID A1, B1, B2) is plotted in a histogram (Fig. 6). The fractional differences are rather small (less than 10%), being less than 2.6% for the 2 MKIDs from wafer and less than 3.3% for those from wafer 2. The maximum change found in \( \delta f_r/f_{r,A2} \) for A1-B1 is \( 2.6 \times 10^{-2} \) and for A2-B2 is \( 3.3 \times 10^{-2} \). These values are higher in comparison with the value reported of \( 1.1 \times 10^{-2} \) for identical resonators of TiN built through sputtering (the resonators are on the same wafer and same MKID).

To verify if the changes of the resonance frequencies are a consequence of the variation of the critical temperature, we analyze the local kinetic inductance of all 48 resonators through the methods of Appendix C. In the case of the local kinetic inductance \( L_{k,i} \), the values are between 18 pH/sq and 24 pH/sq (Fig. 11), where each resonator has a unique value of \( L_{k,i} \). Calculating the global kinetic inductance \( L_{k,g} \) using equation (C1), the values are 19.5 pH/sq, 20.4 pH/sq, 21.5 pH/sq, 22.13 pH/sq for B1, A1, B2, A2, respectively. Then, we obtained a change in \( T_c \) of 0.5 K for A1 respect to A2 and 0.1 K for A1,B1 and A2,B2 considering that \( L_k \propto 1/T_c \). Those values are bigger in comparison with the expected values obtained through the fit to the fractional resonance frequency change, given in table I. Therefore, the variation in the resonance frequency could be due to other factors such as the variation in the losses of the system and in the over-etch into silicon.

In a resonator the losses of the system are counted by the loaded quality factor \( Q_l \). From Fig. 7 it is clear that each resonator has a different \( Q_l \), and in the half of them its value is below the one obtained from the simulation. The fact that the loaded quality factor results lower than the simulated value indicates that there are more losses in the system. These could be by the wire bonding, the connection with the ports and other external agents. In contrast, the values above the designed value could be produced by the CPW line. If we observe the Fig. 4 the variation of the \( S_{12} \) dB presented in the baseline is produced by a mismatch with the CPW line and its connections.

In order to explain any possible process involved in the fabrication stages, we performed three simulations, changing, 1) the area of the resonators by \( \pm 10\% \) (including the CPW and all the components), 2) the dielectric permeability of the substrate (from 68% to 171%) and 3) the non-homogeneity of the etch (depth from 0 to 150 \( \mu m \)). In all the simulations the kinetic inductance used was 21 pH/sq and, in 2) and 3) the Erel was taken as 11.7.

![Fig. 6: Distribution of \( \delta f_r/f_{r,A2} \).](image)

![Fig. 7: Distribution of \( \log_{10}(Q_l) \) for the 48 resonators. The dashed red lines correspond to the minimum and maximum loaded quality factors for the groups with high \( Q_l \) and low \( Q_l \).](image)

V. CONCLUSIONS

We have demonstrated the uniformity of Atomic Layer Deposition through measuring the critical temperature of 48 resonators of TiN. Indistinguishability in the critical temperature in resonators from the same process and a difference of \( 66 \) mK between different process are obtained. In this way, ALD significantly improves the non-uniformity issues in the critical temperature for the fabrication of the MKIDs and superconducting devices. However, in spite of the uniformity, we found a bigger variation in the resonance frequencies in comparison with sputtering. In the same way, the variations of the loaded quality factor are completely unpredictable in each resonator and complicated to control. As a future work, we will investigate the process that affects both parameters.
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Appendix A: Fitting $S_{12}$

In this appendix, we discuss how to obtain the resonance frequency and loaded quality factor from a resonator. Equation (1) contains 7 parameters and two terms, one associated to the environment and the other to the properties of the resonator. The environment term accounts for the contributions to the off-resonance frequencies of $S_{12}$. This term depends on a complex constant $r$ accounting for the gain and phase shift through the system and $\tau$ describing the cable delay. The environment is analytically modeled as a Fourier series expansion but, in our case, we take only the first term because we are taking data around the minimum. Terms of higher order are not necessary as they are used to model all the cable in a bigger range.

To obtain the values of the resonance frequency and loaded quality factor of each resonator we fit the measured transmission amplitude $S_{12}^{data}$ with equation (1) by minimizing the function

$$
\chi^2 = \sum_{n=0}^{N} \frac{|S_{12}(f_n) - S_{12}^{data}(f_n)|^2}{\sigma_n^2},
$$

(A1)

where $\sigma_n^2$ is the associated error in each point of $S_{12}$ obtained from the network analyzer.

Equation (1) depends on the initial values of the seven parameters and $\sigma_n^2$. To calculate $\sigma_n$, we do a new smoothed curve where each point is defined as the mean of the $2n$ nearest neighbors ($n = 8$ in our case). The associated error is computed as the root median square (rms) around the mean. We observe that the data fluctuations lay between the error curves.

We use different methods to determine the initial values of the seven parameters. The values of $a$ and $\tau$ are obtained by doing a fit to the environment term $a \exp(-2\pi j f \tau)$, in ranges outside the resonance frequency. The initial value of the resonance frequency is the point in the complex plane of $S_{12}$ with maximum phase velocity. The initial values of the loaded quality factor and $\phi$ are obtained via the -3 dB method and the phase vs frequency method, respectively.

In Fig. 8 we observe that the resonance frequency of the data appears above the baseline and the same for the bandwidth $\Delta f$. Due to our resonators have an asymmetry in the transmission amplitude $S_{12}$ dB, the resonance frequency is not in the minimum and the $\Delta f$ is not at -3 dB respect to the baseline. In Fig. 9 the $f_r$ is always in the point with maximum phase velocity and the bandwidth divides the circle by the half. These properties are observed in all the resonators, independently if they are simulated or experimentally measured.

We use TMINUIT with the initial values of all parameters to obtain the resonance frequency and loaded quality factor for each resonator. Next, we define the error of the fit as

$$
\sigma_{error} = |S_{12}^{data}(min(f_n))| - |S_{12}(min(f_n))|.
$$

(A2)

In this way, we can establish that two or more resonators are identical if the difference between their resonance frequencies is lower than their maximum $\sigma_{error}$.
TABLE I: Resonance frequencies and loaded quality factors for the 12 resonators of the 4 MKIDs considered in this work.

| Resonator | $f_{\text{data}}^{\text{A1}}$ (GHz) | $Q_l \times 10^3$ | $f_{\text{data}}^{\text{A2}}$ (GHz) | $Q_l \times 10^3$ | $f_{\text{data}}^{\text{B1}}$ (GHz) | $Q_l \times 10^3$ | $f_{\text{data}}^{\text{B2}}$ (GHz) | $Q_l \times 10^3$ |
|-----------|------------|----------------|------------|----------------|------------|----------------|------------|----------------|----------------|
| 10        | 1.0697     | 147.6         | 1.0967     | 74.8           | 1.0207     | 103.0         | 1.0376     | 44.7          |
| 4         | 1.1038     | 3.6           | 1.1408     | 10.1           | 1.0645     | 8.0           | 1.0869     | 31.7          |
| 12        | 1.2868     | 31.1          | 1.3148     | 84.8           | 1.2160     | 54.7          | 1.2275     | 155.8         |
| 3         | 1.3136     | 32.2          | 1.3495     | 4.0            | 1.2487     | 8.0           | 1.2813     | 3.2           |
| 7         | 1.5594     | 165.6         | 1.6073     | 61.0           | 1.5113     | 89.4          | 1.5516     | 46.5          |
| 5         | 1.6116     | 8.4           | 1.6532     | 10.0           | 1.5312     | 10.5          | 1.5620     | 3.5           |
| 11        | 1.9603     | 104.3         | 2.0037     | 35.0           | 1.8603     | 95.6          | 1.8872     | 232.6         |
| 2         | 1.9890     | 1.9           | 2.0482     | 16.6           | 1.9212     | 6.5           | 1.9728     | 7.0           |
| 4         | 2.7363     | 54.4          | 2.8119     | 28.0           | 2.6269     | 26.7          | 2.6826     | 70.8          |
| 8         | 2.7868     | 2.0           | 2.8559     | 4.6            | 2.6691     | 6.5           | 2.6996     | 3.5           |
| 9         | 4.2118     | 80.8          | 4.3164     | 125.7          | 4.0898     | 29.1          | 4.1386     | 55.4          |
| 6         | 4.2970     | 31.8          | 4.4136     | 42.0           | 4.1653     | 6.3           | 4.1821     | 4.6           |

Appendix B: Critical Temperature

To extract the critical temperature through the fractional change of the resonance frequency we perform a chi-squared fit

$$\chi^2 = \sum_{i=1}^n \frac{\left(\frac{\delta f_r(T_i)}{f_r} - \frac{\alpha \sigma_2(T_i, \omega)}{\sigma(0)}\right)^2}{\sigma_{\delta f_r/f_r}^2},$$  \quad (B1)

where the error $\sigma_{\delta f_r/f_r}$ is the median absolute deviation (MAD) and is global. The data set of the MAD is obtained from the error propagation of $\delta f_r(T_i)/f_r(0)$.

FIG. 10: Fractional frequency change $\delta f_r/f_r$ as a function of the temperature for the resonator 2 from the MKID A1 (black) and MKID A2 (blue). The red lines are the fit to equation (2) using the complex conductivity in equation (3).

Appendix C: Kinetic Inductance

From equation (1), we can derive the kinetic inductance of a resonator $L_k$ using the values of $f_r$, $L_g$ and $C_g$. Depending on the design of the resonators, in some cases it is possible to determine the values of $L_g$ and $C_g$ by analytical methods\(^{20}\). However, in our case, it is complicated due to the complexity of the design.

Running a simulation with different values of $L_k$, from 15 pH/sq to 40 pH/sq in steps of 2 pH/sq, we obtained $f_r$ as a function of $L_k$. Then, we did a fit to equation (1) and the values of the geometrical capacitance $C_g$ and geometrical inductance $L_g$ of each resonator were extracted. From the simulation we have identified the 12 resonators and the order in which they appear in the frequency space, which is independent of the value of $L_k$. This allows us to identify to which resonator corresponds each resonance frequency when we analyze the spectrum of the MKID (see Fig. 4).

Fig. 11 shows a histogram of the local kinetic inductance $L_{k_{l}}$ of the 48 resonators derived from the measured $f_r$ and the simulated values of $L_g$ and $C_g$. We can obtain a unique value of the kinetic inductance of all resonators, referred to as global kinetic inductance $L_{k_{G}}$, through finding the value of $L_k$ that minimizes the next
Citations and References

The dashed red lines are the global kinetic inductance extracted from the equation (1) for the 48 resonators.

FIG. 11: Distribution of the local kinetic inductance of the 48 resonators.

In the equation (C1) the sum runs over all 12 resonance frequencies and the error $\sigma_{error}$ is calculated with equation (A2). Fig. 11 shows the values of the global inductance derived with the previous methods.

FIG. 11: Distribution of the local kinetic inductance extracted from the equation (1) for the 48 resonators. The dashed red lines are the global kinetic inductance of each MKID.

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