Simulating the radiation loss of superconducting submillimeter wave filters and transmission lines using Sonnet em

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Abstract. Superconducting resonators and transmission lines are fundamental building blocks of integrated circuits for millimeter-submillimeter (mm-submm) astronomy. Accurate simulation of radiation loss from the circuit is crucial for the design of these circuits because radiation loss increases with frequency, and can thereby deteriorate the system performance. Here, we show a stratification for a 2.5-dimensional method-of-moment simulator Sonnet em that enables accurate simulations of the radiative resonant behavior of submm-wave coplanar resonators and straight coplanar waveguides. The Sonnet simulation agrees well with the measurement of the transmission through a coplanar resonant filter at 374.6 GHz. Our Sonnet stratification utilizes artificial lossy layers below the lossless substrate to absorb the radiation, and we use co-calibrated internal ports for de-embedding. With this type of stratification, Sonnet can be used to model superconducting mm-submm wave circuits even when radiation loss is a potential concern.

Keywords: millimeter-wave; astronomy; simulations; submillimeter-wave; kinetic inductance detectors; integrated superconducting spectrometer.

1 Introduction

Superconducting microwave resonators are used in astronomical instrumentation, quantum computation, and solid-state physics. For designing the resonators and the superconducting transmission line circuit around it, the planar method of moment (MoM) simulation software Sonnet em (Sonnet, hereafter) is widely used. This is because Sonnet requires less simulation time compared to full three-dimensional (3D) simulators (e.g., CST Microwave Studio and HFSS) for planar structures, and it is straightforward to model superconductors in Sonnet.

In recent years, there is an increasing demand in astronomical instrumentation for superconducting circuits that operate in the millimeter-submillimeter (mm-submm) band up to 1 THz. At above ~100 GHz, radiation losses become significant for coplanar structures, and the quality factor of resonators can deteriorate. While full 3D simulators can simulate free-space boundaries, Sonnet requires a perfect electrical conductor (PEC) surface on the four walls perpendicular to the planar structures. This can lead to problems, such as suppression of radiative modes, reflections from the walls back to the circuit, and standing waves. Recently, we have reported that the radiation loss of a straight coplanar waveguide (CPW) can be accurately modeled with Sonnet using a box that is sufficiently large to allow all radiative modes to be excited, and a stratification that prevents reflection from the walls of the simulation box. Here, we present the details of such a simulation and show that the same stratification can also be applied to account for radiation loss in Sonnet simulations of submm wave resonators. We do this by
comparing Sonnet simulations with experiments, and a simulation using CST Microwave Studio (CST, hereafter).

For the Sonnet simulations, we have used Sonnet Version 17.56 on a Windows Server 2019 workstation with two AMD EPYC 7302 16-core processors (3 GHz), with hyper-threading (64 threads in total), and 512 GB of random access memory (16 × 36 GB).

2 Superconducting Submillimeter Wave Resonator

We will study the submm wave resonator shown in Fig. 1. The resonator is a meandering slotline patterned in the superconducting NbTiN ground plane on a $c$-plane sapphire substrate. The second harmonic mode of this resonator at 374.6 GHz is used as one of the bandpass filters in a filter bank circuit of the astronomical spectrometer Deep Spectroscopic High-redshift Mapper (DESHIMA). At this frequency, the filter intercepts the submm wave signal flowing from the input port 1 to the transmission port 2 so that part of the signal is directed to the coupled port 3. The power sent to the coupled port 3 is measured with a microwave kinetic inductance detector (MKID). A previous study of this resonator has shown that, at the resonance frequency, ~13% of the power from the input is radiated into the substrate. This radiative behavior makes it challenging to reproduce these results using Sonnet. Further details about the radiation mechanism of this resonator can be found in Ref. 15.

In Fig. 2, we show the model of the resonator in Sonnet. All slots in the NbTiN film are 2-μm wide. The 100-nm thick NbTiN film is modeled as a metal sheet with a surface inductance of 1 ph/sq, calculated from the resistivity (102 $\mu\Omega$ cm), critical temperature (14.7 K), and thickness (100 nm) of a NbTiN film deposited in an identical manner. (The surface inductance can be calculated from the low-frequency approximation $L_s = R_s/\hbar/(\pi\Delta)$, or more accurately the full Mattis–Bardeen equations, where $R_s$ is the sheet resistance, $\hbar$ is the reduced Planck constant, and $\Delta$ is the superconducting gap energy.) The polyimide blocks under the aluminium bridges have been replaced with a vacuum layer to save computation time. The aluminium film used for the bridges is modeled as a metal sheet with a surface resistance of 0.63 $\Omega$/□. The CPW lines have a characteristic impedance of 93 $\Omega$. The CPW lines extend straight to the ports loaded with a matched impedance. The sapphire substrate is modeled with an anisotropic permittivity of 9.3 in the horizontal directions, and 11.9 in the vertical direction.

In the Sonnet model, all corners in the pattern are sharp, whereas the corners in the real device are rounded with a finite radius of curvature because of optical diffraction in contact mask
In Appendix A, we show that this difference has a negligible effect for the model presented in this article.

3 Sonnet Stratification

3.1 Box

Figure 3 shows the stratification of the ground plane, dielectric layers, and the box around the resonator. In Sonnet, the four sidewalls of the box must be made of PEC. The ceiling and floor are set to the free-space boundary condition. In the horizontal directions, the box is 4096 μm × 4096 μm wide. The box is much larger than the metallization, for the following reasons:

1. When the sidewalls are close to each other, the box behaves like a rectangular waveguide. This means that radiation from the structure will be restricted to the set of discrete
waveguide modes. This can lead to suppression of radiative modes that can be excited if the structure were placed in an infinite space. The typical scale recommended in the Sonnet User’s Guide is one or two times the wavelength.\textsuperscript{7}

2. When the sidewalls are not far enough from the structure, the radiation can be reflected at the walls and couple back into the structure. To prevent this, there must be sufficient attenuation of the signal between the structure and the walls. When standing waves are observed in the current distribution, this is a strong indication that there is significant reflection.

3. The area of the ground plane is kept to the minimum, because the calculation time of Sonnet scales roughly with the number of metal subsections cubed.\textsuperscript{10}

To model an infinite space seen by the structure, we have introduced: (1) a double-layer substrate that is designed to absorb the radiated power without affecting the waves in the resonator and CPWs. Directly under the NbTiN film layer, there is a 100-μm thick layer of sapphire with no dissipative loss. The thickness of 100 μm is much larger than the slot width of 2 μm, ensuring that all the guided waves (near field) are contained in this layer. Under this lossless substrate, there is an artificial lossy substrate that has the same anisotropic permittivity of c-plane sapphire and a loss tangent of tan δ = 0.1. (A smaller loss tangent can be used, in which case the lossy substrate must be thickened to achieve the same attenuation.) The small difference in complex permittivity between the lossless and lossy layers ensures that there is little reflection at the interface. The thickness of the lossy substrate, \( t_{\text{lossy}} \), will be chosen so that the signal radiated from the circuit is strongly attenuated and is not reflected back to the structure. For the same reason, we have also placed an artificial layer of lossy vacuum at 100 μm above the ground plane layer to absorb radiation that is launched above the substrate, depending on the circuit that is modeled. As shown in Sec. 4.5, this layer has no effect for the cases simulated in this paper. Finally, above the lossy vacuum layer and below the lossy substrate, there are 1-mm thick layers of lossless vacuum that separate the lossy layers from the free-space boundaries at the top and bottom of the box. In the experiment, the surface of the lid was covered by carbon-loaded epoxy loaded with SiC grains. The distance from the chip to this surface was \( \sim 10 \) mm.

3.2 \textit{Ports}

Here, we use “co-calibrated internal ports,” because this type of port can be placed on the edge of a metal that is not attached to the Sonnet box. (The most commonly used box-wall port must be attached to the box wall.) The co-calibrated internal ports are de-embedded, so the results are accurate.\textsuperscript{7} For our simulations, we apply a floating ground node connection, which internally creates a generalized local ground (GLG) metal connection at every port.\textsuperscript{7} This GLG metal is removed in the de-embedding process. The short calibration length of 6 μm follows from a private discussion with Sonnet, but it is not studied in detail by us.

4 \textit{Results}

4.1 ‘\textit{Reference}’ \textit{Geometry}

We will first discuss the reference geometry, of which the parameters are given in Table 1. The reference geometry is chosen as a good compromise between accuracy and calculation time. The resonator is placed close to the center of the ground plane, which is 1024-μm wide in both x and y directions. As mentioned earlier, for the NbTiN film in Sonnet, we took a sheet inductance of 1 ph/sq that is derived from measured film properties. However, we adjust the sheet inductance in CST to 0.73 ph/sq to get the resonance frequency close to the measurement. The exact reason for the different sheet inductance required in CST is not clear at the time of publication. Furthermore, to align the simulated resonance frequency to the measurement, we multiplied the Sonnet frequency by a factor of 1.0067, and the CST frequency by a factor of 0.9986.

The S-parameters calculated with Sonnet are compared with CST and measurements in Fig. 4. Because we can only use the MKID at port 3 to measure the power and we do not have
any means to measure the transmitted power to port 2 and the reflected power to port 1, we can obtain only $|S_{11}|^2$ from the measurements. Therefore, we take $|S_{31}|^2$ as the prime indicator for the accuracy of the simulations. Both $|S_{31}|^2$ curves of Sonnet and CST are within the $1\sigma$ error range at the resonance peak.

The time-evolution of the current is a good indication of the presence of standing waves in the simulation box. Figure 5 is a snapshot of an animation (Video 1). The radiation leaving the resonator is not returning to the CPW, and there are no obvious indications of standing waves. (Typically, standing waves are visible if the box is too small, there is not enough dissipation in the box, etc.)
4.2 Sensitivity to Offsets of the Resonator Within the Ground Plane

In Fig. 4, we show the effect of shifting the position of the resonator within the ground plane as shown in Fig. 6 and Table 2. When we take the peak value of $|S_{31}|^2$, the ratio between maximum and minimum of all positions is 1.24 (0.93 dB), which is in many cases an acceptable error tolerance for designing on-chip filters.

Interestingly, the reference position located near the center of the ground plane (hence also the center of the simulation box) yields a peak $|S_{31}|^2$ that is the lowest among all positions. This could be an indication that there remains an effect of a finite distance to the box wall or the ground plane edge. Further investigation in the directions of:

1. moving the ground plane together with the resonator inside the box and comparing the effect, and
2. repeating the simulation with larger box sizes and larger ground plane sizes

are recommended if one would want to further improve the simulation accuracy.

4.3 Sensitivity to the Ground Plane Width

The size of the ground plane can, in general, affect the amount of radiation loss. Here we keep the square shape of the ground plane and vary the length of the sides $w_{GP}$ from 512 to 2048 $\mu$m, as summarized in Table 3. The result is shown in Fig. 7. Compared to the reference geometry ($w_{GP} = 1024 \mu$m), all other values for $w_{GP}$ yield a slightly higher peak $|S_{31}|^2$ value. In general, we expect that the larger the ground plane the more accurate the results are, because we are trying to simulate an infinite ground plane case. However, it should be noted that the experiment was also not with an infinite ground plane; there were neighboring filter channels on both sides of the filter at a distance of $3\lambda/4$. The $|S_{31}|^2$ peak of the smallest, and hence, least accurate $w_{GP} = 512 \mu$m geometry has a $|S_{31}|^2$ peak that is 22% higher than the reference. The $|S_{31}|^2$ peak of the largest, $w_{GP} = 2048 \mu$m geometry has a $|S_{31}|^2$ peak that is 13% higher than the reference.

Fig. 5 Snapshot of the current distribution $J_{xy}$ for the reference geometry. It is worth noting that the current densities plotted do not represent de-embedded data, and therefore areas near any port include the effect of the port discontinuity, according to the manual of Sonnet (Video 1, .mov, 29.7 MB [URL: https://doi.org/10.1117/1.JATIS.8.3.036005.s1]).

Endo et al.: Simulating the radiation loss of superconducting submillimeter wave filters...
Table 2 Parameters defining the set of geometries used to test the sensitivity to offsets of the resonator within the ground plane. Bold characters indicate the reference geometry.

| Parameter                  | Value          |
|---------------------------|----------------|
| $t_{\text{lossySub}}$     | $10^2 \mu m$   |
| $t_{\text{lossyVac}}$     | $10^2 \mu m$   |
| $\tan \delta$            | $10^{-1}$      |
| $w_{\text{GP}}$           | $1024 \mu m$   |
| $\Delta x$                | $-200, -100, 0, +100, +200 \mu m$ |
| $\Delta y$                | $-200, -100, 0, +100, +200 \mu m$ |
| Box size                  | $4096 \mu m \times 4096 \mu m$ |

Table 3 Parameters defining the set of geometries used to test the sensitivity to the ground plane width. Bold characters indicate the reference geometry.

| Parameter                  | Value          |
|---------------------------|----------------|
| $t_{\text{lossySub}}$     | $10^2 \mu m$   |
| $t_{\text{lossyVac}}$     | $10^2 \mu m$   |
| $\tan \delta$            | $10^{-1}$      |
| $w_{\text{GP}}$           | $512, 1024, 1536, 2048 \mu m$ |
| $\Delta x$                | 0              |
| $\Delta y$                | 0              |
| Box size                  | $4096 \mu m \times 4096 \mu m$ |

Fig. 6 Locations of the reference and offset positions on the $1024 \mu m \times 1024 \mu m$ ground plane. The numbers 1–3 indicate the location of the ports.
4.4 Sensitivity to the Thickness of the Lossy Substrate

The thickness of the artificially introduced lossy substrate, \( t_{\text{lossySub}} \), has been varied from 0 to \( 10^4 \) \( \mu \text{m} \), as summarized in Table 4. For the 0 and 1 \( \mu \text{m} \) cases, the adaptive band synthesis of Sonnet had difficulties in converging after simulating at many frequencies, so eventually the simulation had to be terminated. This is most likely because there was a strong standing wave excited in the box because there was not enough attenuation under the ground plane. This shows the necessity to include this lossy layer, and we will focus on the results of \( t_{\text{lossySub}} = 10^1 \) to \( 10^4 \) \( \mu \text{m} \). Figure 8 shows the resonance peak for the different lossy-substrate thicknesses. Except for the case where the lossy substrate is the thinnest, \( t_{\text{lossySub}} = 10^1 \) \( \mu \text{m} \), the results are completely insensitive to varying \( t_{\text{lossySub}} \). This is an additional, strong indication that the waves radiated from the vicinity of the resonator are strongly attenuated by the lossy layer, thereby not returning to the circuit and not creating standing waves that affect the results.

Although large values of \( t_{\text{lossySub}} \) hardly affect the simulation time, we have chosen a minimal value of \( t_{\text{lossySub}} = 10^2 \) \( \mu \text{m} \) as the reference value because it is sufficient.
4.5 Sensitivity to the Thickness of the Lossy Vacuum Layer

In a similar way as the previous section, the thickness of the artificially introduced lossy vacuum layer $t_{\text{lossyVac}}$ has been varied from 0 to $10^4 \mu m$, as summarized in Table 5. The lossy vacuum layer has no noticeable effect on the results in the case of this model, as shown in Fig. 9. The lossy vacuum layer has no effect on the straight-CPW simulation in Sec. 5 either. This is as expected, because the radiation from these circuits is directed toward the substrate. Moreover, even for geometries that might radiate toward the box ceiling, radiation could be efficiently absorbed by the free-space boundary because there is no reflective dielectric-vacuum interface in between. Nevertheless, we include the lossy vacuum layer in the box to confirm that there are no standing waves in the volume above the substrate, by an analysis as shown in Fig. 9.

4.6 Sensitivity to the Cell Size (Meshing)

Finally, we check that the simulation has a sufficiently small cell size (or mesh size). The reference geometry had a cell size of 0.5 $\mu m$ in both $x$ and $y$ directions. In Fig. 10, we compare the

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**Table 5** Parameters defining the set of geometries used to test the sensitivity to the thickness of the lossy vacuum layer. Bold characters indicate the reference geometry.

| Parameter  | Value |
|------------|-------|
| $t_{\text{lossySub}}$ | $10^2 \mu m$ |
| $t_{\text{lossyVac}}$ | $0, 10^1, 10^2, 10^3, 10^4 \mu m$ |
| $\tan \delta$ | $10^{-1}$ |
| $w_{\text{GP}}$ | $1024 \mu m$ |
| $\Delta x$ | 0 |
| $\Delta y$ | 0 |
| Box size | $4096 \mu m \times 4096 \mu m$ |
Making the cell size smaller shifted the resonance frequency downward by a factor of 1.0096. In Fig. 10, we have multiplied the frequency of the 0.25 μm result with this factor so that the resonance frequencies match. After this correction, the two sets of curves are nearly overlapping. This result verifies that the reference geometry is sufficiently meshed.

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**Fig. 9** Effect of changing the thickness of the lossy vacuum layer, \( t_{\text{lossyVac}} \). The three curves for \( t_{\text{lossyVac}} = 10^2 \) μm, \( 10^3 \) μm, and \( 10^4 \) μm are completely overlapping for all three \( S \)-parameters.

**Fig. 10** Effect of changing the mesh size, from the reference value of 0.5 μm (solid curves) to 0.25 μm (dashed curves) in both \( x \) and \( y \) directions.

reference result with a simulation in which the cell size was reduced to 0.25 μm. Making the cell size smaller shifted the resonance frequency downward by a factor of 1.0096. In Fig. 10, we have multiplied the frequency of the 0.25 μm result with this factor so that the resonance frequencies match. After this correction, the two sets of curves are nearly overlapping. This result verifies that the reference geometry is sufficiently meshed.

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### 5 Simulation of Radiation Loss from a Straight CPW

To show the general applicability of the stratification, we present the simulation of radiation loss from a straight CPW using the same stratification as the one used for the resonator. A similar
A simulation has been presented in Ref. 11. Here, we will compare the results to the analytical formula of Ref. 18.

We have used Sonnet to simulate the radiation loss of a straight CPW made of PEC with a center strip width of $2 \mu m$ and a slot width of $2 \mu m$, on a silicon substrate with a relative dielectric constant of 11.44. The lateral dimensions of the Sonnet box were $3000 \mu m \times 3000 \mu m$. The thicknesses of the layers were the same as those of the reference geometry, except for the thickness of the lossy substrate that was varied: $t_{\text{lossySub}} = 10^2, 10^3, 10^4 \mu m$. Figure 11 shows the Sonnet-simulated $S_{21}$ for different CPW lengths. $|S_{21}|^2$ was less than $-45 \text{ dB}$ with no clear frequency-dependence, which proves that the ports are matched well to the CPW line and reflections are negligible for this analysis. From the slope of a linear-fit to the $|S_{21}|^2$ as a function of frequency, we obtain a loss of $0.030 \text{ dB mm}^{-1}$. This is close to the loss of $0.025 \text{ dB mm}^{-1}$ obtained from analytical formula of Frankel et al. as follows:

$$
\alpha_{\text{rad}} = \frac{\pi}{2} \left[ \frac{\sin^4 \Psi}{\cos \Psi} \right] \frac{(s + 2w)^2 \epsilon_r^{3/2}}{c^3 K(\sqrt{1 - k^2}) K(k)} f^3,
$$

where $\alpha$ is the attenuation constant, $\Psi = \arccos(\sqrt{\epsilon_{\text{eff}}/\epsilon_r})$ is the radiation angle (see Fig. 12. 90 deg $-\Psi$ is equivalent to the Mach angle for sonic shock waves), $\epsilon_{\text{eff}}$ is the effective dielectric constant of the CPW mode (defined as $\epsilon_{\text{eff}} \equiv \sqrt{c/v_p}$, where $v_p$ is the phase velocity), $\epsilon_r$ is the relative dielectric constant of the substrate, $s$ is the width of the center strip of the CPW, $w$ is the width of the CPW slots, $c$ is the velocity of light in vacuum, $k = s/(s + 2w)$, $f$ is the frequency, and $K$ is the complete elliptical integral of the first kind. It should be noted that the simulated data has an offset from zero loss at zero distance, most likely due to port discontinuities.

The current distribution around the CPW is shown in Fig. 12 (Video 2). The current propagates away from the CPW, showing no indication of standing waves in the vertical direction. The direction of the shock waves agrees well with $\Psi = \arccos(\sqrt{\epsilon_{\text{eff}}/\epsilon_r}) = 42.5 \text{ deg}$.
Discussion and Conclusion

Our results show that the 2.5-dimensional MoM solver Sonnet can be used to accurately simulate the radiation loss from planar superconducting circuits, placed in between a thick substrate and vacuum. The Sonnet simulations of the resonator reproduce the $|S_{31}|^2$ measurement result to within the error margin of the measurement. The Sonnet results are robust against variations in the geometric parameters, though it appears to be that changing the parameters studied here lead to a small systematic increase in the $|S_{31}|^2$ peak value. This could be an indication that even better accuracy could be reached by studying the effect of the box size and ground plane size, in combination, in greater detail.

Appendix A: Effect of Rounded Corners on the Sonnet Simulation

A potential concern when comparing the Sonnet simulation and the measurement is the resolution of lithography used to fabricate the device. We typically observe that corners that are sharp by design become rounded due to optical diffraction in ultraviolet contact-mask lithography. The radius of curvature of the corners is typically about 0.5 μm, this is also visible in the micrograph shown in Fig. 1.

Here, we have compared two Sonnet models, one with sharp corners and the other with rounded corners. We have modeled each rounded corner with three cells, as shown in Fig. 13(a). This required a mesh size of 0.25 μm. Because of this mesh size, the model with sharp corners is identical to the model with the finer mesh size investigated in Sec. 4.6.

We compare the results of rounded and sharp corners in Fig. 13. The frequencies are shifted by factors of 1.0096 and 0.99955 for the models with sharp and rounded corners, respectively, so that the peak frequencies match. It is natural that the resonance frequency is slightly different, because the rounding slightly shortens the effective electrical length of the slot. After correcting for this small frequency shift, the results are indistinguishable.

This result indicates that the rounding of corners does not have a significant effect on the conclusions in the main article about radiation loss.
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