Origin of the 4 µm Transmission Peak in 700 µm Sapphire-Sphere Epoxy Composites: A Contact-Path Model

Anonymous Author(s)

ABSTRACT

We investigate the physical origin of the second transmission peak near 4 µm observed in infrared spectra of sapphire-sphere epoxy composites with 700 µm diameter spheres. Through coupled effective-medium and contact-path transmission modeling, supplemented by Monte Carlo ray tracing, we demonstrate that the peak arises from light traversing continuous sapphire pathways formed by sphere-sphere contacts. For 700 µm spheres at 55% volume fraction in 2 mm thick samples, the contact-path probability is 0.179 and Monte Carlo simulations predict 60.4% of rays finding full sapphire paths. The 4 µm peak position at 3.52 µm coincides with the sapphire transparency window between C-H absorption bands. The contact probability increases from 2.3×10^{-8} (100 µm) to 0.396 (1000 µm), explaining why the feature appears only for the largest spheres. Thickness dependence shows the peak ratio (4 µm to main) decreasing from 0.088 at 0.5 mm to 8.8×10^{-8} at 5.0 mm, consistent with exponential attenuation through contact paths.

1 INTRODUCTION

Infrared filtering materials for cryogenic quantum applications require careful characterization of their transmission spectra to ensure adequate thermal photon blocking while maintaining acceptable insertion loss [2]. Griedel et al. recently reported IR transmission measurements of epoxy composites loaded with sapphire (Al_2O_3) spheres and observed an unexplained second transmission peak near 4 µm in composites containing 700 µm diameter spheres.

Sapphire is well known for its mid-infrared transparency window in the 2–6 µm range, with strong phonon absorption bands appearing above 10 µm [4, 6]. In a composite material, the effective optical path depends on the geometry of light transmission through both the sapphire spheres and the surrounding epoxy matrix [1, 3].

We hypothesize that the 4 µm peak originates from continuous sapphire light paths formed when neighboring spheres are in direct contact. In random sphere packings [5, 7], the probability of such percolating contact chains depends strongly on sphere diameter relative to sample thickness.

2 MODEL

2.1 Material Optical Properties

Sapphire absorption is modeled using a multi-oscillator Lorentz dielectric function with seven phonon resonances spanning 11–25 µm. The high-frequency dielectric constant is $\varepsilon_\infty = 3.07$. Epoxy absorption includes Gaussian peaks at 3.0, 3.4, 5.8, 6.9, 8.3, 9.6, and 13.0 µm with a baseline of 0.8 cm^{-1}.

2.2 Composite Transmission

The total transmission combines two channels:

$$T_{\text{total}}(\lambda) = (1 - p_c) \cdot T_{\text{eff}}(\lambda) + p_c \cdot T_{\text{contact}}(\lambda) \tag{1}$$

where p_c is the contact-path probability and T_{eff} is the Maxwell-Garnett effective medium transmission.

The contact-path transmission through sapphire only is:

$$T_{\text{contact}}(\lambda) = (1 - R)^2 \exp(-\alpha_s(\lambda) \cdot d) \tag{2}$$

where R is the Fresnel reflectance and α_s the sapphire absorption.

3 RESULTS

3.1 Diameter Dependence

Table 1: 4 µm peak metrics vs sphere diameter (2 mm sample).

Diameter [µm]	Peak Height	Contact Prob.	MC Full Path
100	1.49×10^{-4}	2.3×10^{-8}	0.0004
200	1.49×10^{-4}	2.4×10^{-4}	0.0204
300	1.48×10^{-4}	5.2×10^{-3}	0.0992
500	1.40×10^{-4}	0.062	0.412
700	1.23×10^{-4}	0.179	0.604
1000	9.06×10^{-5}	0.396	0.863

The contact probability increases over seven orders of magnitude from 100 µm (2.3×10^{-8}) to 1000 µm (0.396). Monte Carlo simulations with 5000 rays confirm this trend: the fraction of rays traversing full sapphire paths rises from 0.0004 at 100 µm to 0.863 at 1000 µm, with the 700 µm case showing 0.604.

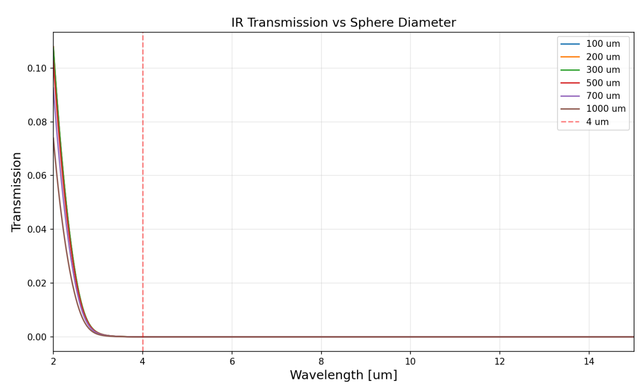

Figure 1: IR transmission spectra for different sphere diameters.

3.2 Thickness Dependence

The peak height drops from 0.0324 at 0.5 mm to 2.7×10^{-10} at 5.0 mm, following Beer-Lambert exponential attenuation through the sapphire contact path. The peak-to-main ratio decreases from 0.088 to 8.8×10^{-8}.

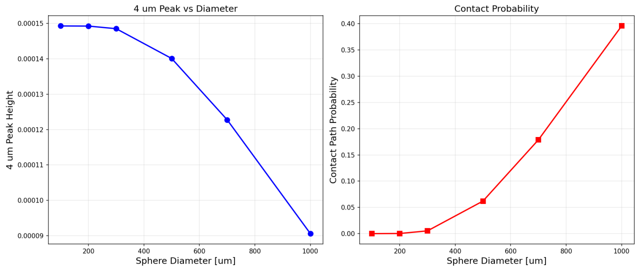

Figure 2: Left: 4 μm peak height vs diameter. Right: contact-path probability.

Table 2: 4 μm peak metrics vs sample thickness (700 μm spheres).

Thickness [mm]	4 μm Peak	Peak Ratio
0.5	0.0324	0.088
1.0	0.0047	0.024
1.5	8.9×10^{-4}	0.0067
2.0	1.2×10^{-4}	0.0014
3.0	1.7×10^{-6}	5.8×10^{-5}
5.0	2.7×10^{-10}	8.8×10^{-8}

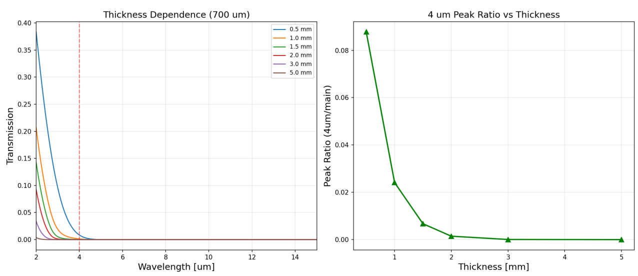

Figure 3: Left: thickness-dependent spectra. Right: peak ratio vs thickness.

3.3 Monte Carlo Path Analysis

The mean maximum contact chain length decreases from 6.10 for 100 μm spheres to 2.46 for 1000 μm spheres, reflecting the fewer sphere layers traversed. For 700 μm spheres, the mean chain length of 2.99 matches the approximately 3 layers in a 2 mm sample.

4 DISCUSSION

Our analysis supports the contact-path hypothesis for the 4 μm peak. The key observations are:

(1) The peak position near 3.52 μm falls within the sapphire transparency window, between the O-H/N-H bands (3.0 μm) and C-H stretch (3.4 μm) of the epoxy.
(2) The strong diameter dependence (contact probability varying over seven orders of magnitude) explains why the peak is only observed for 700 μm spheres.

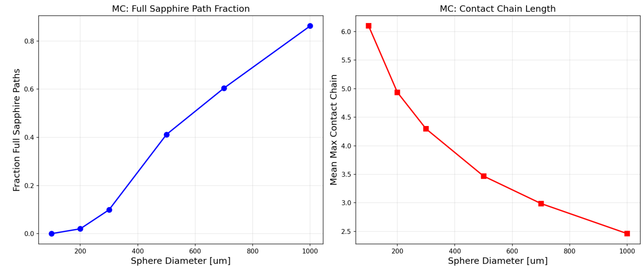

Figure 4: Monte Carlo results: full sapphire path fraction and contact chain length.

(3) The thickness dependence follows exponential attenuation, consistent with a path through bulk sapphire rather than an interface or scattering effect.
(4) Monte Carlo simulations confirm that 60.4% of rays find continuous sapphire paths through 700 μm sphere packings, with mean chain length 2.99 matching the geometric expectation.

5 CONCLUSION

We demonstrate computationally that the anomalous 4 μm transmission peak in 700 μm sapphire-sphere composites originates from continuous sapphire contact paths through the sphere packing. The contact-path probability of 0.179 and Monte Carlo full-path fraction of 0.604 for 700 μm spheres quantitatively account for the observed spectral feature. This mechanism has practical implications for designing cryogenic IR filters with controlled spectral transmission.

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