

# A Theoretical Study On The Electrodynamics Properties Of Superconducting Ultra-Thin Films And Their Optical Response In The Terahertz Domain

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## Abstract

*Superconducting ultra-thin films exhibit distinctive electrodynamics behaviour governed by reduced dimensionality, Cooper-pair condensation, and the formation of an energy gap at the Fermi level. This paper presents a theoretical investigation into the optical conductivity and THz-frequency response of conventional metallic superconducting thin films, with niobium nitride (NbN) and tantalum nitride (TaN) as primary model systems. The Mattis–Bardeen (MB) theoretical framework within BCS formalism is adopted to analyse real ( $\sigma_1$ ) and imaginary ( $\sigma_2$ ) components of complex conductivity across the 0.1–1.1 THz spectral window. The central hypothesis posits that as film thickness diminishes below the London penetration depth ( $\lambda_L$ ), disorder-induced modifications to the superconducting gap produce measurable deviations from BCS-predicted optical responses. Secondary datasets from terahertz frequency-domain spectroscopy (THz-FDS) experiments are reanalysed to validate theoretical predictions. Results demonstrate that NbN films of 3.9–5.0 nm exhibit  $T_c$  suppression, penetration depth enhancement, and spectral weight redistribution consistent with disorder-driven pair-breaking, while TaN films adhere closely to weak-coupling BCS predictions. These findings carry implications for the rational engineering of kinetic inductance detectors, superconducting nanowire single-photon detectors, and quantum sensing platforms.*

**Keywords:** Superconducting ultra-thin films, THz optical conductivity, Mattis–Bardeen theory, London penetration depth, kinetic inductance detectors

## 1. Introduction

The intersection of superconductivity and terahertz (THz) spectroscopy has emerged as one of the most productive domains in condensed matter physics over the past two decades. Superconductors are characterised by the formation of Cooper pairs and the appearance of an energy gap  $2\Delta$  near the Fermi level. In conventional metallic superconductors, typical gap energies correspond to photon frequencies of 0.3–1.5

THz, placing them squarely within the THz spectral window (0.1–10 THz). This alignment makes THz techniques a uniquely sensitive, non-contact probe of Cooper-pair density, quasiparticle dynamics, and the London penetration depth all central quantities in quantitative superconductivity research. Ultra-thin superconducting films, those with thicknesses comparable to or smaller than the superconducting coherence length ( $\xi$ ) or London penetration depth ( $\lambda_L$ ), represent a technologically critical and physically rich class of materials. In these systems, dimensionality reduction modifies the electronic density of states, increases the role of disorder scattering, and introduces two-dimensional (2D) phase-fluctuation effects such as the Kosterlitz–Thouless–Berezinskii (KTB) transition collectively altering the THz optical response in ways that deviate from bulk BCS predictions. Understanding these deviations is essential both for fundamental condensed matter physics and for the design of next-generation quantum sensors.

NbN and TaN thin films have served as canonical model systems in this context. Their critical temperatures lie in the 5–16.5 K range, their gap frequencies fall within the THz window ( $\sim 0.4$ – $1.2$  THz), and they can be deposited with precise thickness control by reactive DC magnetron sputtering (Pracht et al., 2013; Liu et al., 2024). Cai et al. (2023) refined the theoretical framework for extracting optical conductivity from THz data using an improved Tinkham-based model that accounts for incident angle, polarisation, and multiple substrate reflections a methodological advance directly applicable to ultra-thin film characterisation. The theoretical foundation for interpreting THz data rests on the Mattis–Bardeen (MB) formalism (Mattis & Bardeen, 1958), which calculates complex conductivity via thermally activated quasiparticle contributions and across-gap pair-breaking transitions. The Tinkham relation links film THz transmission to sheet conductivity, enabling experimental extraction of  $\sigma_1(\omega)$  and  $\sigma_2(\omega)$  (Tinkham, 1956). Optically driven superconductors such as those studied by Wang et al. (2023) in  $K_3C_{60}$  additionally illustrate how non-equilibrium THz responses can

probe the condensate far from equilibrium, motivating deeper theoretical understanding of linear optical response as a baseline. This paper systematically examines the theoretical framework governing THz electrodynamics in ultra-thin superconducting films, analyses secondary experimental data within a unified BCS/MB framework, and quantifies the consequences of film thickness and disorder for optical response.

## 2. Literature Review

The foundational framework for superconductor optical spectroscopy was established by Tinkham (1956), whose energy-gap interpretation of far-infrared transmission experiments on superconducting films provided the first experimental confirmation of the BCS gap, and by Mattis and Bardeen (1958), whose formalism for anomalous skin effect in superconductors remains the dominant paradigm for THz optical data interpretation. Zimmermann et al. (1991) extended MB theory to arbitrary electron purity from the clean limit ( $\ell \gg \xi_0$ ) to the dirty limit ( $\ell \ll \xi_0$ ) enabling quantitative modelling of disordered thin films that could not otherwise be described. The Ferrell–Tinkham–Glover sum rule, established by Ferrell and Glover (1958), constrained the redistribution of optical spectral weight across the superconducting transition, connecting superfluid density to measurable integrated conductivity. Experimental progress in THz superconductor spectroscopy accelerated with the development of THz frequency-domain spectroscopy (THz-FDS) using backward-wave oscillators (BWOs). Dressel et al. (2008) provided a comprehensive review of THz techniques applied to conventional metallic superconductors including Nb and nitrides, highlighting the sensitivity of these approaches to gap structure, quasiparticle scattering rates, and the coherence peak in  $\sigma_1$ . The more general review by Dressel (2013) synthesised theoretical and experimental knowledge of microwave-to-infrared electrodynamics, establishing the interpretive framework for optical gap measurements in metallic thin films.

The landmark study by Pracht et al. (2013) applied THz-FDS across 0.09–1.1 THz to ultra-thin NbN ( $d = 3.9\text{--}4.7$  nm) and TaN ( $d = 4.9\text{--}5.1$  nm) films on sapphire substrates. These authors demonstrated that TaN films at their measured disorder levels are well described by BCS theory with  $2\Delta/kBT_c \approx 3.52$ , while NbN films begin to deviate systematically a signature of incipient superconductor-insulator transition (SIT) behaviour. Pracht et al. (2012) had earlier reported the direct THz spectroscopic observation of the

superconducting gap in a TiN thin film, confirming the validity of MB-based gap extraction from sub-gap transmission suppression. Beck et al. (2011) investigated energy-gap dynamics in NbN thin films using time-resolved THz spectroscopy, measuring an ultrafast gap recovery timescale of approximately 2.5 ps following optical quasiparticle injection a finding critically relevant to SNSPD switching speed. Basov and Timusk (2005) reviewed THz-to-infrared electrodynamics of high- $T_c$  superconductors, demonstrating that optical spectroscopy provides model-independent access to superfluid density and quasiparticle scattering rates in both conventional and unconventional superconductors. The on-chip THz spectrometer of Potts et al. (2023) extended these measurements to NbN films narrower than 7.5  $\mu\text{m}$  below 2% of the Rayleigh diffraction limit demonstrating gap signatures across the superconducting transition in device-scale geometries. Studies targeting penetration depth and dimensionality effects in NbN were consolidated by Poláčková et al. (2023), who quantified  $\lambda_{GL}(0)$  values of 430, 250, and 140 nm for 10, 50, and 100 nm NbN films respectively, and established that orbital effects dominate the upper critical field in moderately thick films. Bretz-Sullivan et al. (2022) reported high kinetic inductance NbTiN transmission line resonators in the ultra-thin film limit, connecting film disorder to microwave/THz energy dissipation. Torras-Coloma et al. (2024) demonstrated superconducting nitridised-aluminium films with controllable  $T_c$  and low THz loss, providing a new material platform for quantum circuits. Nagai et al. (2024) presented a simplified THz spectroscopic ellipsometry approach using sheet conductivity analysis for ultra-thin films, validated on nickelate perovskites across 78–478 K. Šindler et al. (2024) provided deeper theoretical insight into NbN THz response under applied magnetic fields, showing that the Herman–Hlubina model with pair-conserving and pair-breaking scattering reproduces Faraday-geometry conductivity data more accurately than standard MB theory. Ahn and Nagaosa (2021) demonstrated theoretically that clean multi-band superconductors with broken inversion symmetry or finite spin-orbit coupling permit intrinsic momentum-conserving optical excitations representing the frontier beyond the MB dirty-limit paradigm.

## 3. Objectives

1. To theoretically analyse the frequency-dependent complex optical conductivity ( $\sigma_1, \sigma_2$ ) of ultra-thin NbN and TaN superconducting films within the Mattis–Bardeen/BCS framework across the 0.1–1.1 THz

spectral range and evaluate deviations from BCS predictions as a function of film thickness and disorder level.

- To assess the interrelationship among film thickness, critical temperature, London penetration depth, energy gap, and condensate spectral weight using experimentally validated secondary data, with direct implications for THz-sensitive quantum device applications.

#### 4. Methodology

This study employs a theoretical-analytical research design combined with secondary data analysis drawn from peer-reviewed THz spectroscopic studies of NbN and TaN ultra-thin films. No new experimental data are generated. The primary theoretical framework is the Mattis–Bardeen formalism, in which  $\sigma(\omega) = \sigma_1(\omega) - i\sigma_2(\omega)$  is calculated from BCS density of states and Fermi–Dirac occupation functions at finite temperature. For films in the dirty limit (mean free path  $\ell \ll \xi_0$ ), the Zimmermann et al. (1991) extension

accommodating arbitrary scattering rate ( $1/\tau$ ) is adopted. The Tinkham thin-film transmission relation  $T(\omega) = (1 + n_{\text{sub}})/(1 + n_{\text{sub}} + Z_0 d \sigma)$ , where  $n_{\text{sub}} \approx 3.1$  for sapphire at THz frequencies and  $Z_0$  is the free-space impedance, connects optical conductivity to measurable transmission amplitude. The sample set comprises NbN films ( $d = 3.9\text{--}100$  nm) and TaN films ( $d = 4.9\text{--}5.1$  nm) deposited by reactive DC magnetron sputtering on R-plane sapphire substrates. Critical temperatures are obtained from four-probe dc resistance–temperature measurements; spectral analysis spans 0.09–1.1 THz ( $3\text{--}37$  cm<sup>-1</sup>). Data for all tables are drawn exclusively from traceable, DOI-verified published sources. Quantitative comparison of theoretical predictions and experimental outcomes evaluates BCS validity and identifies disorder-induced deviations.

#### 5. Results

**Table 1: Thickness-Dependent Superconducting Parameters of NbN Films**

Film Thickness $d$ (nm)	Critical Temp. $T_c$ (K)	Resistivity $\rho_n$ ( $\mu\Omega \cdot \text{cm}$ )	London Pen. Depth $\lambda_{GL}(0)$ (nm)
3.9	7.2	~400	~500
4.5	12.8	~370	~445
5.0	11.2	~360	~420
10.0	13.5	360	430
50.0	15.3	210	250
100.0	15.8	80	140

Source: Pracht et al. (2013); Poláčková et al. (2023)  
Table 1 presents the thickness-dependent evolution of fundamental superconducting parameters in NbN films. As thickness decreases from 100 nm toward ~4 nm,  $T_c$  suppresses progressively from 15.8 K to 7.2 K while normal-state resistivity rises and London

penetration depth increases sharply. This inverse relationship between  $d$  and  $\lambda_{GL}(0)$  reflects increasing kinetic inductance in the ultra-thin film limit, consistent with Pracht et al. (2013) and corroborated by Poláčková et al. (2023).

**Table 2: Real ( $\sigma_1$ ) and Imaginary ( $\sigma_2$ ) Optical Conductivity of NbN at 0.5 THz ( $d \approx 4.5$  nm,  $T_c = 12.8$  K)**

Temperature $T/T_c$	$\sigma_1$ ( $\times 10^4 \Omega^{-1} \text{m}^{-1}$ )	$\sigma_2$ ( $\times 10^4 \Omega^{-1} \text{m}^{-1}$ )	$\sigma_1/\sigma_N$
0.99 (just above $T_c$ )	2.8	0.0	1.00
0.90	3.1	1.4	1.11 (coherence peak)
0.70	2.1	3.6	0.75
0.50	0.8	5.2	0.29
0.30	0.2	6.8	0.07

Source: Adapted from Pracht et al. (2013); Dressel (2013)

Table 2 illustrates the temperature-dependent evolution of  $\sigma_1$  and  $\sigma_2$  at 0.5 THz. The coherence peak in  $\sigma_1$  at  $T/T_c = 0.90$  rising ~11% above normal-state value is a direct signature of thermally activated

quasiparticle transitions as theorised by the MB formalism (Pracht et al., 2013). With decreasing temperature,  $\sigma_1$  collapses as Cooper pairs condense, while  $\sigma_2$  rises continuously, representing the growing reactive kinetic inductance response of the condensate (Dressel, 2013).

**Table 3: BCS Gap Ratio ( $2\Delta/k_B T_c$ ) for NbN and TaN Ultra-Thin Films**

Material	$d$ (nm)	$T_c$ (K)	$2\Delta(0)$ (meV)	$2\Delta/k_B T_c$	Gap Frequency $\nu_g$ (THz)	Disorder $kF\ell$
NbN	4.7	14.5	4.35	$3.49 \pm 0.08$	1.05	4.5–5.5
TaN	5.0	8.6	2.60	$3.51 \pm 0.06$	0.63	~5.0
TaN	4.9	5.8	1.75	$3.52 \pm 0.05$	0.42	~5.2
NbN	3.9	7.2	2.00	$3.23 \pm 0.12$	0.48	~4.2
NbN (bulk)	—	16.5	4.96	3.49	1.20	—

Source: Pracht et al. (2013)

Table 3 shows the BCS gap ratio for NbN and TaN films. TaN films adhere closely to the weak-coupling BCS prediction of 3.52 regardless of thickness, validating the MB description at moderate disorder.

NbN films at  $d = 3.9$  nm show the ratio dropping to 3.23, indicating disorder-driven pair-breaking with Ioffe–Regel parameter  $kF\ell$  falling to ~4.2 approaching the regime of anomalous metallic behaviour as documented by Pracht et al. (2013).

**Table 4: THz Transmission Ratio ( $T_s/T_n$ ) vs. Frequency for NbN Film ( $d = 4.5$  nm,  $T_c = 12.8$  K)**

Frequency (THz)	$T_s/T_n$ at $T/T_c = 0.50$	$T_s/T_n$ at $T/T_c = 0.70$	$T_s/T_n$ at $T/T_c = 0.90$
0.1	0.72	0.85	0.97
0.3	0.78	0.88	0.96
0.5	0.83	0.91	0.94
0.7	0.91	0.95	0.96
0.9	0.97	0.98	0.99
1.1	1.00	1.00	1.00

Source: Adapted from Pracht et al. (2013)

Table 4 presents theoretical THz transmission ratios ( $T_s/T_n$ ) as a function of frequency. A clear spectral threshold is visible: suppression is strongest at low frequencies and vanishes above the gap frequency  $\nu_g \approx 1.05$  THz (Pracht et al., 2013). At  $T/T_c = 0.50$ , the

condensate screens low-frequency THz fields most effectively, producing maximum suppression at 0.1 THz. These trends are directly predicted by the Tinkham thin-film relation and confirm the BCS energy gap as the physical origin of sub-gap opacity.

**Table 5: London Penetration Depth, Coherence Length, and 2D Phase Transition Signatures in NbN**

$d$ (nm)	$T_c$ (K)	$\lambda_L(0)$ (nm)	$\xi_0$ (nm)	Regime	KTB Signature
3.0	~5.5	~600	~4.5	2D	Yes
5.0	11.2	~420	~4.8	2D	Yes
6.5	13.0	~370	~4.9	2D–3D crossover	Marginal
10.0	13.5	430	~5.0	Near-2D	No
50.0	15.3	250	~4.5	3D	No

Source: Pracht et al. (2013); Poláčková et al. (2023)

Table 5 illustrates the evolution of penetration depth and phase-transition character with film thickness. Films at  $d \leq 6.5$  nm display Kosterlitz–Thouless–Berezinskii (KTB) signatures a 2D superfluid phase governed by vortex–antivortex pair unbinding rather than uniform gap suppression. At  $d \geq 10$  nm, the

system crosses into 3D BCS behaviour. Importantly,  $\lambda_L \gg d$  throughout, validating the Tinkham thin-film approximation and confirming effective 2D electrodynamics for all ultra-thin cases (Pracht et al., 2013).

**Table 6: Sheet Resistance, Kinetic Inductance, and Condensate Spectral Weight for NbN Films at 4.2 K**

$d$ (nm)	$T_c$ (K)	$R_{sq}$ ( $\Omega/\square$ )	$Lk$ (pH/ $\square$ )	$SW_s/SW_n$ (%)	$\nu_g$ (THz)
6	~8.3	~1200	~28.0	~88	~0.48
12	~12.7	~620	~12.0	~91	~0.73
24	~13.8	~340	~6.5	~94	~0.85

48	~14.6	~185	~3.1	~97	~1.05
124	14.63	~55	~0.9	~99	~1.20

Source: Glowacka et al. (2014); corroborated by Bretz-Sullivan et al. (2022)

Table 6 presents sheet resistance, kinetic inductance, condensate spectral weight, and gap frequency as functions of NbN film thickness. Thinner films exhibit dramatically elevated kinetic inductance from  $\sim 0.9$   $\mu\text{H}/\square$  at 124 nm to  $\sim 28$   $\mu\text{H}/\square$  at 6 nm a parameter critical to KID and SNSPD engineering (Bretz-Sullivan et al., 2022). The reduced condensate spectral weight fraction (88% at  $d = 6$  nm vs.  $\sim 99\%$  at  $d = 124$  nm) indicates that a measurably larger portion of normal-state spectral weight has not condensed into the superfluid in ultra-thin films, directly impacting detector responsivity.

## 6. Discussion

The results of this theoretical study provide a coherent, multi-parameter picture of the THz electrodynamics properties of superconducting ultra-thin films, directly addressing both objectives. The frequency-dependent complex conductivity of NbN and TaN films has been mapped within the MB framework, and the interplay among film thickness, penetration depth, gap ratio, and condensate spectral weight has been quantified against verified experimental data. A central and unambiguous finding is that TaN ultra-thin films ( $\sim 5$  nm), even at considerably reduced thickness, conform closely to BCS weak-coupling predictions, with  $2\Delta/k_{\text{BTc}} \approx 3.52$  (Table 3) and transmission curves well reproduced by the Zimmermann MB formalism (Pracht et al., 2013). This result isolates disorder rather than dimensionality reduction per se as the primary driver of anomalous optical response. NbN films at  $d = 3.9$  nm, by contrast, show a gap ratio of  $3.23 \pm 0.12$ , reflecting that their lower Ioffe–Regel parameter ( $kF\ell \approx 4.2$ ) places them closer to the Mott–Anderson localisation boundary where disorder-enhanced pair-breaking and incipient superconductor-insulator transition physics begin to manifest. This distinction carries a fundamental lesson: thickness suppression of  $T_c$  and gap energy in NbN is disorder-mediated, not a pure confinement effect as might naively be assumed from the data in Table 1 alone.

The coherence peak in  $\sigma_1$  just below  $T_c$  rising  $\sim 11\%$  above normal-state conductivity at  $T/T_c = 0.90$  (Table 2) is a direct experimental validation of case-2 coherence factors in MB theory, reflecting constructive interference of thermally excited quasiparticle transitions across the gap (Dressel, 2013). The progressive transfer of spectral weight

from  $\sigma_1$  into the condensate delta function manifested as rising  $\sigma_2$  with decreasing temperature is quantitatively consistent with the Ferrell–Tinkham–Glover spectral weight sum rule (Ferrell & Glover, 1958). This confirms that spectral weight is conserved across the transition, concentrated at zero frequency in the superfluid condensate, with no unaccounted losses in the studied disorder range. The penetration depth data (Table 5) reveal a physically critical transition at  $d \approx 6.5$  nm. Below this thickness, KTB-type 2D phase fluctuations dominate, causing superfluid density to collapse via vortex–antivortex unbinding above  $T_{\text{KTB}}$  rather than through the mean-field pair-breaking mechanism assumed by standard BCS/MB theory. This explains the nonlinearity in  $\sigma_2(T)$  curves at low temperatures in the thinnest NbN films, and means that for  $d < 6.5$  nm, a purely mean-field MB analysis will overestimate the condensate density and mispredict the temperature dependence of THz transmission a finding directly relevant to device modelling. Beck et al. (2011) confirmed the ultrafast 2.5 ps gap recovery timescale in NbN, which is set by the quasiparticle recombination rate and is critically thickness-dependent, impacting maximum count rates in SNSPDs.

The kinetic inductance scaling in Table 6 has direct quantitative implications for quantum device engineering. The  $\sim 31\times$  increase in  $Lk$  as film thickness decreases from 124 nm to 6 nm provides a controllable, reproducible route to high-inductance resonators required by kinetic inductance detectors and superconducting qubits, without necessitating geometrically narrow nanowires (Bretz-Sullivan et al., 2022). However, the concomitant reduction in condensate spectral weight fraction from  $\sim 99\%$  to  $\sim 88\%$  means that a larger fraction of quasiparticle excitations from incident photons does not recombine into the condensate, increasing recombination-noise contributions. Potts et al. (2023) demonstrated that this trade-off can be evaluated directly on sub-diffraction NbN patterned structures using on-chip THz spectroscopy, enabling device-level characterisation of  $Lk$ ,  $\sigma_1$ , and  $\sigma_2$  simultaneously. The theoretical advances by Šindler et al. (2024) demonstrating that the Herman–Hlubina model with pair-conserving and magnetic pair-breaking disorder improves upon standard MB theory for NbN films in applied magnetic fields indicate that any future extension of this analysis to SNSPD operation in external fields or THz modulator applications will require beyond-MB

formalisms. Similarly, the work of Ahn and Nagaosa (2021) on clean multi-band superconductors identifies the conditions under which inversion symmetry breaking or spin-orbit coupling introduces direct optical transitions forbidden by standard BCS momentum-conservation arguments, pointing toward an emerging frontier where MB theory is insufficient. The results presented here establish the clean BCS/MB baseline indispensable as a reference for such extensions. The connection to optically driven nonlinear superconductivity explored by Wang et al. (2023) further underscores the importance of well-characterised equilibrium electrodynamics properties as a foundation for nonlinear THz physics in these film systems.

### 7. Conclusion

This theoretical study has systematically characterised the THz-domain electrodynamics properties of ultrathin NbN and TaN superconducting films within the Mattis–Bardeen/BCS framework. Films in the 5–100 nm range exhibit BCS-consistent gap structure, coherence peaks, and spectral weight redistribution. TaN films adhere closely to weak-coupling predictions regardless of thickness, isolating disorder as the key driver of anomalous behaviour in NbN. Films below approximately 6.5 nm enter a 2D phase-fluctuation regime governed by KTB physics beyond mean-field theory. Kinetic inductance scales inversely and strongly with thickness, at the cost of reduced condensate spectral weight. These results provide a rigorous theoretical foundation for co-optimising film thickness, disorder, and THz optical response in quantum sensor design KIDs, SNSPDs, and kinetic inductance resonators where these parameters are not independently tunable.

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