

FE-NEGF for Cryogenic Thermal Management

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Abstract—Thermal transport in cryogenic electronic and quantum-device interconnects can depart strongly from the diffusive regime assumed in Fourier theory. We use a finite-element nonequilibrium Green's function (FE-NEGF) approach to calculate coherent phonon transmission and thermal conductance in a realistic Au/Nb/Au/In/Au/Nb/Au flip-chip contact, where In (indium) forms the solder joint and superconducting Nb suppresses electronic heat conduction. We first compare the complete coherent stack with a series construction in which the central In layer is treated as an equilibrium reservoir. The two descriptions are not equivalent: the artificial reservoir removes phase and mode correlations and underestimates the conductance of the coherent full stack. We then investigate the dependence on the In-layer thickness. At 0.1 K, reducing the In thickness from 2500 to 10 nm increases the conductance by approximately 30%. This low-temperature dependence arises because the dominant acoustic phonons have wavelengths much larger than the thickness of a thin In layer and therefore do not fully resolve it as an extended propagation region. As the temperature increases, shorter-wavelength phonons increasingly resolve the two Au/In interfaces, while integration over a broader spectral window averages the thickness-dependent phase contributions. Consequently, the conductance becomes only weakly dependent on the In thickness, provided that a finite In layer remains present. These results highlight both the non-additive nature of coherent cryogenic heat transport and the dominant role of interface mode matching in the higher-temperature part of the investigated regime.

Index Terms—thermal management, cryogenic temperature, finite-element, non-equilibrium Green's function, flip-chip.

I. INTRODUCTION

Thermal management is a major challenge in cryogenic electronics and quantum-device integration [1]–[3], where small parasitic heat loads can raise the local temperature and degrade device performance [4]. This issue is particularly important in flip-chip architectures, in which qubit and control chips operating at different temperatures are connected through nanoscale or microscale multilayer contacts [5]. At sub-kelvin and few-kelvin temperatures, the dominant phonon wavelengths and mean free paths can become comparable to, or larger than, the characteristic dimensions of these interconnects [6]. Heat transport may then depart strongly from the local diffusive behavior assumed in Fourier theory.

In this regime, a multilayer contact cannot necessarily be represented as a sequence of independent thermal resistances. Such a description implicitly assumes that each internal layer

can be assigned a local temperature and that phonons re-thermalize between successive interfaces. When propagation remains ballistic and phase coherent, however, an internal layer is part of a single scattering region rather than an equilibrium reservoir. The conductance is then controlled by the global phonon transmission of the complete structure, including mode conversion, multiple reflections, and interference across the successive interfaces.

A suitable description must therefore combine realistic device geometries with open-boundary wave transport. Finite-element nonequilibrium Green's function (FE-NEGF) theory provides such a framework [7]. The finite-element discretization accommodates material inhomogeneity and complex geometries, while the Green's function formalism describes coherent phonon propagation and coupling to external thermal reservoirs.

In this work, we apply FE-NEGF to phonon transport of a realistic Au/Nb/Au/In/Au/Nb/Au flip-chip contact, where In represents the solder joint and superconducting Nb suppresses electronic heat conduction [8]. We first compare the coherent conductance of the complete multilayer with a series construction in which the central In layer is treated as an artificial equilibrium reservoir. We show that the two descriptions are not equivalent and that the series-resistance approximation underestimates the coherent conductance. We then investigate the dependence on the In thickness. At very low temperature, the dominant acoustic phonon wavelengths can greatly exceed the thickness of a thin In layer, producing a pronounced thickness dependence of the conductance. With increasing temperature, the broader spectral transport window averages the thickness-dependent phase contributions, and the conductances of structures containing a finite In layer progressively converge.

II. FINITE-ELEMENT NON-EQUILIBRIUM GREEN'S FUNCTION METHOD

The finite-element nonequilibrium Green's function (FE-NEGF) method combines a continuum description of elastic waves with an open-system treatment of coherent phonon transport. As summarized in Fig. 1, the device geometry is discretized using finite-element shape functions, yielding the global mass and stiffness matrices $\mathbf{M}$ and $\mathbf{K}$. Spatially dependent densities and elastic tensors allow the different materials and interfaces of the multilayer structure to be represented within the same mesh. Perfectly bonded interfaces

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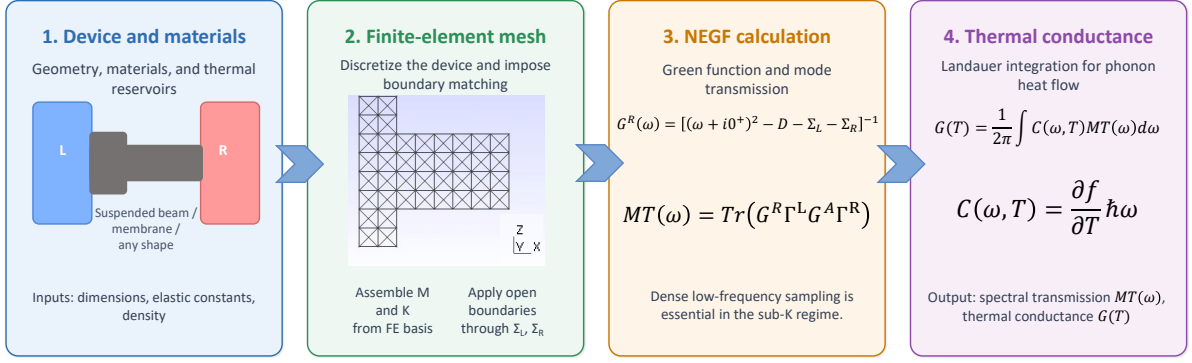


Fig. 1. **Finite-element NEGF workflow for sub-kelvin phonon transport.** The geometry and material parameters are discretized using finite elements to obtain the mass and stiffness matrices. Open boundaries are introduced through the lead self-energies, and the phonon transmission is evaluated from the device Green's function. The thermal conductance is then obtained by Landauer integration, with dense low-frequency sampling in the sub-kelvin regime.

are described by shared nodal degrees of freedom, enforcing displacement continuity and traction balance.

The calculation is performed in mass-normalized coordinates using the dynamical matrix

$$\mathbf{D} = \mathbf{M}^{-1/2} \mathbf{K} \mathbf{M}^{-1/2}. \quad (1)$$

The structure is partitioned into a finite central region C connected to left and right semi-infinite leads. Their effect is incorporated through the retarded self-energies $\Sigma_\alpha^r = \mathbf{D}_{C\alpha} \mathbf{g}_\alpha^r \mathbf{D}_{\alpha C}$, where $\mathbf{g}_\alpha^r$ is the surface Green's function of lead $\alpha = L, R$. The retarded Green's function of the open device is

$$\mathbf{G}^r(\omega) = [(\omega + i\eta)^2 \mathbf{I} - \mathbf{D}_C - \Sigma_L^r(\omega) - \Sigma_R^r(\omega)]^{-1}, \quad (2)$$

where $\eta \rightarrow 0^+$ imposes the retarded boundary condition. Defining $\Gamma_\alpha = i(\Sigma_\alpha^r - \Sigma_\alpha^a)$ and $\mathbf{G}^a = (\mathbf{G}^r)^\dagger$, the elastic phonon transmission is obtained from the Caroli expression

$$\mathcal{T}(\omega) = \text{Tr} [\mathbf{G}^r \Gamma_L \mathbf{G}^a \Gamma_R]. \quad (3)$$

This formulation includes multiple reflections, mode conversion, interference, and coupling to the external reservoirs throughout the complete scattering region.

In the linear-response regime, the thermal conductance is calculated from the Landauer expression

$$G(T) = \frac{1}{2\pi} \int_0^\infty \hbar \omega \frac{\partial n_B(\omega, T)}{\partial T} \mathcal{T}(\omega) d\omega, \quad (4)$$

where $n_B = [\exp(\hbar\omega/k_B T) - 1]^{-1}$. Because the thermal weighting function is concentrated at low frequencies in the sub-kelvin regime, a dense frequency grid is used near $\omega = 0$. Convergence is checked with respect to the mesh, frequency sampling, and numerical parameter η .

The calculations assume harmonic elastic dynamics, perfectly bonded interfaces, and phase-coherent phonon propagation. Anharmonic scattering, structural disorder, and internal thermalization are not included. An internal layer therefore remains part of the coherent scattering region unless an additional reservoir self-energy is explicitly introduced.

III. RESULTS AND DISCUSSION

We apply the FE-NEGF method to the vertical flip-chip [5] contact shown in Fig. 2. The contact consists of an Au/Nb/Au/In/Au/Nb/Au multilayer connecting a low-temperature qubit chip to a higher-temperature CMOS stage. The In layer represents the solder joint, while the superconducting Nb layers suppress the electronic contribution to heat transport [8]. The present calculation focuses on the coherent phonon contribution. The outer Au regions are coupled to the left and right thermal reservoirs.

A. Breakdown of the series-resistance picture

A conventional thermal-resistance description would divide the symmetric structure into two nominally identical half-stacks, each extending from an external Au reservoir to the central In layer. If the In layer is assumed to be an equilibrium reservoir, the two half-stack conductances combine in series according to

$$G_{\text{series}}(T) = \left[\frac{1}{G_{\text{half}}(T)} + \frac{1}{G_{\text{half}}(T)} \right]^{-1} = \frac{G_{\text{half}}(T)}{2}. \quad (5)$$

Equivalence between the coherent full-stack calculation and this series model would therefore require $G_{\text{half}}(T) = 2G_{\text{full}}(T)$.

Figure 3 shows that this relation is not satisfied. Over most of the relevant frequency range, $2\mathcal{T}_{\text{full}}(\omega)$ is larger than $\mathcal{T}_{\text{half}}(\omega)$. After Landauer integration, this gives

$$G_{\text{full}}(T) > G_{\text{series}}(T) = \frac{G_{\text{half}}(T)}{2}. \quad (6)$$

Thus, inserting an equilibrium reservoir at the center of the In layer underestimates the conductance of the coherent structure.

The discrepancy arises because introducing the intermediate reservoir is not simply an algebraic decomposition of the same device. It changes the physical boundary conditions: phonons reaching the reservoir lose their phase and mode information and are re-emitted with an equilibrium Bose-Einstein distribution. In the full-stack calculation, by contrast, the In layer

Vertical contact in flip-chip

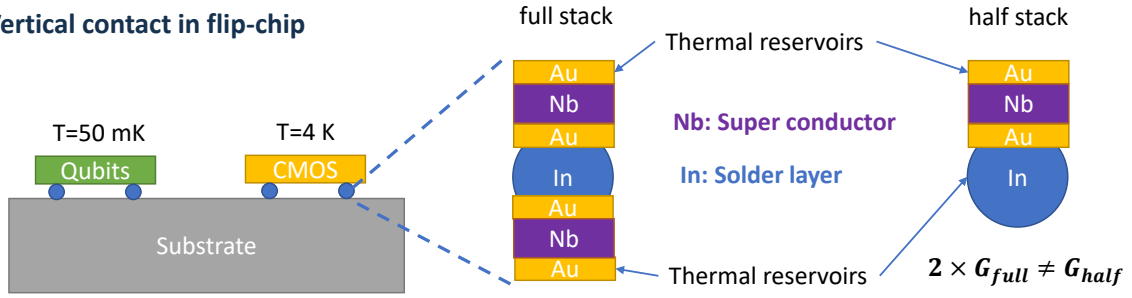


Fig. 2. **Vertical flip-chip contact and transport partitions.** A qubit and CMOS chips are connected to a substrate through an Au/Nb/Au/In/Au/Nb/Au multilayer contact. In the coherent calculation, the complete multilayer is treated as a single scattering region coupled only to the two external thermal reservoirs. In the series construction, the system is divided into two half-stacks by introducing an artificial equilibrium reservoir in the central In layer.

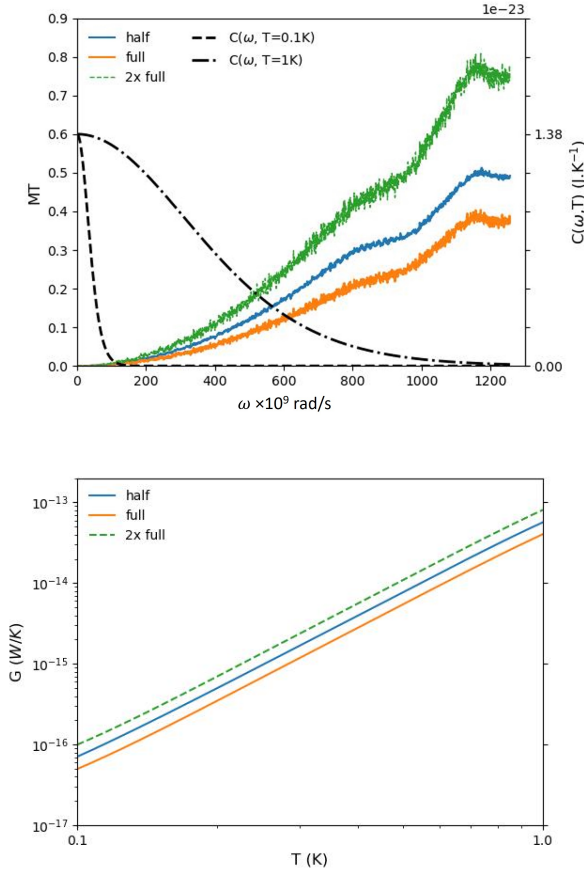


Fig. 3. **Breakdown of the series-resistance description.** Top: phonon transmissions of the coherent full stack and of a half-stack terminated by an equilibrium reservoir. The curve $2T_{full}(\omega)$ is included as a guide to the series condition $G_{half} = 2G_{full}$ after Landauer integration. The dashed and dash-dotted curves show the thermal weighting function $C(\omega, T) = \hbar\omega \partial n_B / \partial T$ at 0.1 and 1 K. Bottom: corresponding thermal conductances. The coherent full-stack conductance exceeds the series estimate $G_{half}/2$, demonstrating that the intermediate In layer cannot be treated as a thermal reservoir in the coherent regime.

remains part of a single coherent scattering region. Phonons propagate across the complete multilayer while retaining the correlations generated by reflection, mode conversion, and interference at the successive interfaces. The conductance is therefore determined by the global mode matching of the complete stack rather than by a sum of local layer resistances.

The Landauer kernels included in Fig. 3(top) further show that the conductance below 1 K is dominated by the low-frequency part of the transmission spectrum. The non-additivity observed in this frequency range is consequently directly relevant to sub-kelvin operation.

B. Effect of the In-layer thickness

We then vary the In thickness l while keeping the remaining layers unchanged. Figure 4 shows the resulting conductance and the normalized ratio

$$r_l(T) = \frac{G_l(T)}{G_{2500 \text{ nm}}(T)}, \quad (7)$$

where the $l = 2500 \text{ nm}$ structure is used as the reference.

The thickness dependence is strongest at the lowest temperatures. At 0.1 K, the conductance of the $l = 10 \text{ nm}$ stack is approximately 30% larger than that of the reference structure, whereas the enhancement is approximately 10% for $l = 50 \text{ nm}$ and only a few percent for $l = 1000 \text{ nm}$. As the temperature approaches 1 K, the conductance of all structures containing a finite In layer converge toward the reference value. The structure with $l = 0$, however, remains clearly separated and has a conductance approximately 40–50% larger over the investigated temperature interval.

The low-temperature thickness dependence can be understood by comparing l with the wavelength of the thermally occupied acoustic phonons. Using the transverse-acoustic sound velocity of In, $v_{TA} = 1032 \text{ m s}^{-1}$, the condition $\lambda = l$ defines the frequency $f_l = v_{TA}/l$. For $l = 10 \text{ nm}$, $f_l \simeq 103 \text{ GHz}$. The characteristic thermal frequency and wavelength may be estimated as

$$f_T \sim \frac{k_B T}{h}, \quad \lambda_T \sim \frac{\hbar v_{TA}}{k_B T}. \quad (8)$$

At $T = 0.1\text{--}0.2 \text{ K}$, this gives $f_T \simeq 2.1\text{--}4.2 \text{ GHz}$ and $\lambda_T \simeq 250\text{--}500 \text{ nm}$. These wavelengths are much larger

than a 10 nm In layer. Equivalently, the propagation phase accumulated across the In layer,

$$\phi(f, l) = ql = \frac{2\pi fl}{v_{TA}}, \quad (9)$$

is small for the phonons dominating transport at 0.1–0.2 K. The thin In region therefore does not behave as an extended propagation layer. Instead, it acts as a subwavelength elastic element whose response is closer to that of a very thin junction than to that of the 2500 nm reference.

This does not imply that the thin In layer is completely invisible: the acoustic mismatch and mode conversion at the Au/In interfaces remain present. Rather, the small value of ql limits the additional phase accumulated during propagation inside In layer and therefore weakens the thickness-dependent interference associated with the layer interior.

As the temperature increases, phonons with larger frequencies and shorter wavelengths enter the Landauer transport window. The phase ql then becomes appreciable, and the In layer is increasingly resolved as a propagation region. At the same time, the conductance is integrated over a broader frequency interval containing both constructive and destructive interference contributions. The observed convergence of the finite-thickness curves is consistent with this spectral averaging: the integrated conductance becomes progressively less sensitive to the precise phase accumulated across the In layer and more strongly controlled by the common interface and mode-matching properties of the stack.

The $l = 0$ result must be interpreted separately. Removing In eliminates the two Au/In interfaces and changes the material sequence, rather than merely reducing the propagation phase inside In. The corresponding structure therefore remains distinct even when the conductances of the finite-thickness stacks become nearly independent of l .

IV. CONCLUSION

We have applied FE-NEGF to coherent phonon transport through an Au/Nb/Au/In/Au/Nb/Au flip-chip contact at sub-kelvin temperatures. The conductance of the complete multilayer is not reproduced by dividing the structure into two half-stacks and treating the central In layer as an equilibrium reservoir. Introducing such a reservoir removes phase and mode correlations and therefore changes the physical transport problem, leading to an underestimate of the coherent full-stack conductance. We further showed that the conductance depends strongly on the In thickness at the very low temperatures. For thin In layers, the dominant acoustic phonon wavelengths greatly exceed the layer thickness, so that the layer acts as a subwavelength elastic element rather than as an extended diffusive region. As temperature increases, the broader transport window averages the thickness-dependent phase contributions, and the conductance of the finite-thickness structures progressively converge. These results demonstrate that cryogenic multilayer contacts must be treated through their global phonon transmission rather than as simple networks of local thermal resistances, and identify solder-layer thickness as a relevant design parameter for cryogenic interconnects.

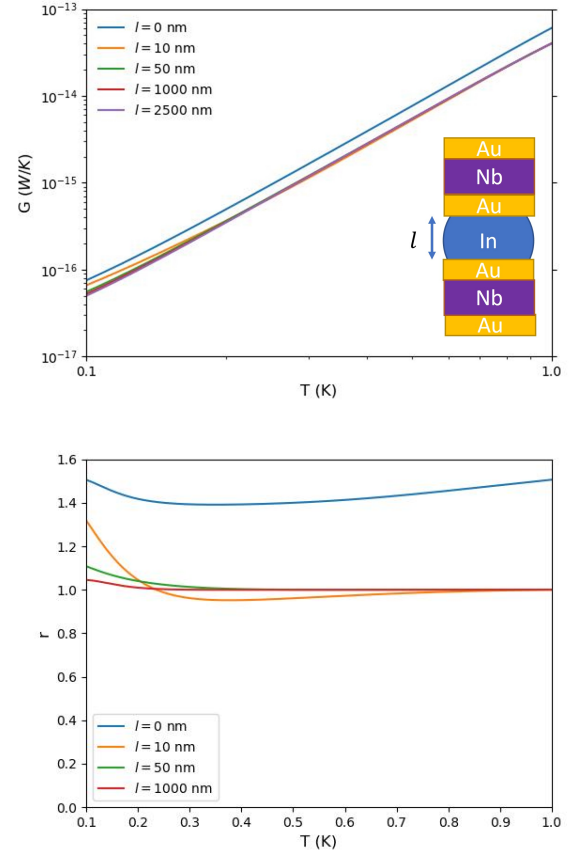


Fig. 4. **Effect of the In-layer thickness on coherent thermal transport.** Top: thermal conductance $G_l(T)$ for $l = 0, 10, 50, 1000$, and 2500 nm. The inset defines the varied In thickness. Right: conductance ratio $r_l(T) = G_l(T)/G_{2500 \text{ nm}}(T)$. The thickness dependence is most pronounced at low temperature, where the dominant phonon wavelengths exceed the thickness of the thin In layers. The conductances of the finite-thickness stacks converge with increasing temperature, whereas the $l = 0$ structure remains distinct because the Au/In interfaces are absent.

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