DOI: 10.54254/2753-8818/2025.GL24876

Phonon-based Thermal Boundary Resistance Models for Micro- and Nanoscale Devices

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Abstract. Micro and nano-semiconductor devices are increasingly crucial in multiple fields such as information technology and artificial intelligence. However, as the volume of transistors decreases and their density increases, local heat accumulation occurring in devices due to the Joule heating effect seriously affects their service life and performance. Therefore, thermal management of devices has become more and more important. As a key factor limiting heat dissipation, thermal boundary resistance (TBR) is particularly significant in nanoscale devices, accounting for over 50% of the total thermal resistance. The theoretical models of thermal boundary resistance can not only help accurately predict the thermal boundary resistance but also effectively understand its influence mechanism. This paper selects and introduces some typical classic theoretical models, elaborates on their characteristics and limitations, summarizes various influencing factors of thermal boundary resistance and provides an outlook on the future research of thermal boundary resistance.

Keywords: Micro and nano- nano-semiconductor devices, Thermal boundary resistance, Theoretical models, Phonon

1. Introduction

With the development of science and technology, micro- and nano semiconductor devices play a key role in many fields such as information technology and artificial intelligence. Moore's Law states that current transistor processes enable tens of billions of transistors to be aggregated over a $1cm^2$ area of the device.

However, as transistors decrease in size and increase in density, these transistors are bound to develop huge a amount of heat when operating at high frequencies,which comes mainly from the Joule heat of the current inside the device. Joule heat generates a localized heat build-up, leading to an increase in device temperature, which seriously affects device performance. At the same time, increasingly miniaturized devices also create problems such as impeded heat dissipation and concentrated thermal stress, providing challenges for device thermal management[1].

Studies have shown that thermal boundary resistance(TBR) accounts for over 50% of the total thermal resistance in nanoscale devices, particularly in the microscale (<100 nm), where its contribution to overall thermal conductivity exhibits exponential growth. Structural and material differences between the two sides of the interface lead to heat accumulation at the interface.

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Therefore, this paper mainly focuses on the thermal boundary resistance mentioned in the article by Cheng et al. The concept of thermal boundary resistance is derived from the temperature difference between the two sides of the interface, and we define the thermal boundary resistance as the ratio of the temperature difference between the two sides of the interface (ΔT) to the density of heat flow through the interface (Q) [2]

Concerning what is proposed in general heat transfer, we can similarly consider that the thermal boundary conductance (TBC) is the reciprocal of the thermal boundary resistance, and the two are inversely correlated.

In solid state physics, we describe lattice vibrations that propagate energy in the form of waves in terms of a quasiparticle phonon. Heat conduction in micro- and nano-devices needs to be studied from a phonon perspective because their dimensions are close to or smaller than the phonon mean free path, leading to a significant enhancement of phonon scattering. The frequent scattering of phonons, as quantized energy units of lattice vibrations, triggered by interfaces, defects and structural disorder at the micro- and nano-scale, dramatically shortens the phonon transport path and reduces the thermal conductivity. At this time, the traditional continuous medium model fails, and it is necessary to study the thermal conductivity behavior based on the phonon transport mechanism to provide theoretical support for the thermal management of devices. [3]The methods to study the phonon transport at the interface include model analysis, Boltzmann transport equation and molecular dynamics.

This article is based on the classical models for estimating interface thermal resistance: the acoustic mismatch model (AMM) and, diffuse mismatch model. As listed in Table 1, this article is introduced from the classical models for estimating thermal boundary resistance: acoustic mismatch model (AMM) and diffuse mismatch model (DMM)and focuses on the recent research on the models related to thermal boundary resistance under the respective influencing factors and calculation methods, summarize the characteristics of each method, and put forward prospects for future research.

The article will primarily introduce the following models: Acoustic Mismatch Model (AMM) [4],Diffuse Mismatch Model (DMM)[4] ,Mixed Mismatch Model (MMM)[5], Joint Frequency Diffuse Mismatch Model(JFDMM)[6], Two Temperature Model (TTM)[7].

Table 1: Introduction to various models

factor	Model Name And Abbreviation	Core Modifications
roughness	Acoustic Mismatch Model (AMM)	The classic model that considers an extremely smooth interface
roughness	Diffuse Mismatch Model (DMM)	The classic model that considers an extremely disordered interface
roughness	Mixed Mismatch Model (MMM)	summary of the two classic roughness models
temperature	Joint Frequency Diffuse Mismatch Mode (JFDMM)	models considering temperature and inelastic scattering
electron-phonon coupling	Dual Temperature Model (TTM)	models considering electron-phonon coupling and heat transfer pathways
Phonon distribution mismatch	N/A	N/A

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2. Classic AMM and DMM models

The assumptions made by the Acoustic Mismatch Model (AMM) and Diffuse Mismatch Model (DMM) are mainly based on two extremes of interfacial roughness, where the AMM assumes that there is only transmission and reflection for interfacial phonon conduction, while the DMM, at the other extreme, assumes that only diffuse scattering of phonons occurs. Both models give a calculation of the interfacial phonon transmittance by assuming that the interface is at the extremes of smoothness and roughness, respectively; if the interfacial phonon transmittance is high, it means that more phonons can pass through the interface and continue to propagate, which increases the phonon thermal conductivity, and vice versa, if the interfacial phonon transmittance is low, the phonons are more likely to be reflected or scattered, resulting in a lower phonon thermal conductivity.

AMM essentially views phonon transmission as a continuous wave[4], with only specular reflection and refraction of phonons occurring at smooth interfaces, Within the AMM framework, phonon transport is simplified as a continuous wave process . When phonons encounter a smooth interface, their behavior resembles optical specular reflection and refraction: incident phonons are partially reflected back into the original medium and partially transmitted into the adjacent medium, with the reflection and transmission angles governed by acoustic refraction law.

At this point the phonon transmission coefficient can be found

$$\alpha_{AMM,A-B} = \frac{4Z_A Z_B}{(Z_A+Z_B)^2} \tag{1}$$

The phonon transmittance of the DMM then assumes that the phonons undergo diffuse scattering and that the interface is in an extremely disordered and rough situation. The transmittance depends only on the phonon density of states D, in this "fully disordered interface" scenario, the phonon transmission process resembles random collisions between gas molecules, with the transmittance coefficient quantified by Equation (2). This reflects how differences in phonon density of states directly influence energy transfer efficiency.

At this point the phonon transmission coefficient is found

$$\alpha_{DMM,A-B} = \frac{\sum_j D_{BV_{Bj}}}{\sum_j D_{AV_{Aj}} + \sum_j D_{BV_{Bj}}} \tag{2}$$

However, both models can only simulate the thermal boundary resistance at low temperatures, which is different from the experimental situation at high temperatures[8]. Therefore, this paper gives a follow-up study on the two factors of roughness and temperature.

3. Roughness

Based on the original AMM and DMM, the impact of surface roughness on the interface and thermal boundary conductance can be understood. At the microscopic level, surface roughness refers to the micro-scale unevenness of the interface caused by local variations in atomic arrangement, which affects the density of states at the interface as well as phonon scattering and transmission. However, the assumptions made by the AMM and DMM are both at the extreme boundary cases. Therefore, in 2018, Zhang et al. proposed a modified mismatch model- the mixed mismatch model (MMM)[5], which presents a new way of calculating phonon transmittance based on AMM and DMM, based on the classical model. MMM weights AMM/DMM results via specularity parameter p.

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That is, the scattering of phonons at the boundary is considered to include both models as a linear summation of the phonon transmittances of the two models, and p is a specularity parameter, the smaller the interface the rougher it is [9,10].

Under the prediction calculation of MMM, for the At/Si interface, the predicted data were compared with the simulated data of molecular dynamics (MD), and both of them were well matched, indicating that the model is somewhat accurate in predicting the thermal resistance of interfaces with arbitrary roughness [9].

Zong et al. not only compared this with the simulation results, but also carried out further experiments to measure the thermal conductance of the At/Si interface, and found that it matches the predicted results.

4. Temperature and inelastic scattering

None of the existing models that consider the roughness can accurately predict the thermal boundary resistance of micro- and nanodevices at high temperatures due to the fact that unlike at low temperatures where elastic scattering dominate, these models neglect the effect of inelastic scattering conduction of phonons on the thermal boundary resistance at high temperatures [8].Therefore, recent studies on the influence of temperature as well as inelastic scattering on the thermal boundary resistance are given below.

To clarify the effect of temperature, it is first necessary to clarify the relationship between temperature and inelastic scattering. The studies and calculations of Kelires et al. point out that as the temperature increases, probability of phonon inelastic scattering increases greatly[11].The increased probability of inelastic scattering of phonons at high temperatures is not consistent with the predictive models given previously. In 2024, Chen et al. showed that inelastic phonon scattering affects the thermal conductivity through a complex mechanism, including changing the phase space in which the phonons scatter and affecting the interfacial coupling, thus exhibiting different transport properties in different frequency ranges[12]. Studies such as these imply that temperature and inelastic scattering are also among the key influences on thermal boundary resistance.

The dividing temperature between the dominance of elastic and inelastic scattering of phonons can generally be judged by the Debye temperature T_D REF _Ref200101298 \r \h [8] . This is because inelastic scattering usually requires a large exchange of energy between the phonons, while at low temperatures, the phonon energy itself is small, and it is difficult for significant energy transfer to occur to achieve inelastic scattering. Therefore, in the T< T_D temperature interval, phonon elastic scattering plays a dominant role. Similarly, when the temperature is much higher than the Debye temperature T_D , most of the atoms in the crystal are excited to higher vibrational energy levels, the energy of phonons is higher, and the inelastic scattering between phonons becomes very frequent. At this time, the phonon inelastic scattering plays a dominant role.

To study and predict the effect of inelastic scattering on the thermal resistance of the interface at high temperature, this paper focuses on Hopkins et al. 2007 proposed a joint frequency vibration model JFDMM (joint frequency diffuse mismatch model) [6] based on DMM, JFDMM consider the effect of inelastic scattering, that the DMM assumed by the There is only one frequency of phonons, and the same frequency of elastically scattered phonons are emitted during heat conduction. It is pointed out that the phonon transport at the interface of JFDMM will be affected by the joint frequency vibration on both sides of the interface, and the frequency of the phonons is not certain, and the given thermal conductivity, h_{BD} is calculated by the equation

DOI: 10.54254/2753-8818/2025.GL24876

$$h_{BD} = \frac{1}{4}\sum_j v_{mod,j}\int_0^{\omega^c_{mod,j}} \alpha_1(\omega)\hbar_\omega D_{mod,j}(\omega)\frac{\partial n(\omega,T)}{\partial T}d\omega \quad (3)$$

where $v_{mod,j}$ is the phonon velocity corrected to take into account the joint vibration at the interface, $\omega^c_{mod,j}$ is the corrected cut-off frequency taking into account the joint vibration modes near the interface, α1(ω) is the phonon transmittance, $\hbar_\omega = \frac{h_\omega}{2\pi}$,h is Planck's constant, $D_{mod,j}(\omega)$ is the density of phonon states, and $\frac{\partial n(\omega,T)}{\partial T}$ is the partial derivative of the Bose-Einstein distribution function concerning temperature.

Comparing the model predictions with the experimentally measured thermal conductivity of the Bi, Pb/diamond interface by Lyeo and Cahill et al.[13], and the experimentally measured thermal conductivity of Au/diamond by Stoner and Maris et al. [14], it is found that the JFDMM matches the experimental data better compared to the DMM.

Although JFDMM can predict the thermal boundary resistance better, it still has a large error in more complicated scattering cases[8]. For this reason, in 2023, Hu et al. also gave a new model MHHIM based on DMM[15], MHHIM accurately predicted the thermal boundary resistance of GaN/AIN, and further put forward the effect of the temperature on the thermal boundary resistance, pointing out that the temperature will increase the contribution of high-frequency phonons and decrease the contribution of low-frequency phonons. The contribution of high-frequency phonons decreases, and the contribution of low-frequency phonons increases.

In addition, there are classical models such as the Maximum Transmission Model (MTM) to describe the effects of inelastic scattering.

5. Electron-phonon coupling

In addition to the transport of phonons itself (elastic and inelastic scattering), electron-phonon coupling also has some influence on the thermal boundary conductivity. 2021 Quan et al. summarized the effects of electron-phonon coupling under thermal equilibrium and non-equilibrium conditions by reviewing the research on the aspects related to the thermal boundary transport of electron-phonon coupling in recent years[16].

To specifically elucidate the effect of electron-phonon coupling at the interface, Majumdar et al. proposed the two-temperature model (TTM)[7] in 2004, but due to the complexity of the computational simulation, the article mainly focuses on the improvement of the TTM by Li et al. in 2015 [17].Li et al. classified the interfacial heat transport by electron-phonon coupling into three pathways: Phonon-only Conduction , Interface Electron-Phonon Coupling, Metallic Electron Conduction + Interface Phonon Scattering

By comparing the thermal boundary conductance predicted by the model formulation with three sets of experiments, namely, Pb-diamond interface, Ti-diamond interface, and TiN-MgO interface, it is found that the predicted and experimental values are closer to each other, which is a better indication of the accuracy of the TTM.

6. Phonon distribution mismatch

In addition to the above cases, recent studies have also shown that, in addition to conventional phonon scattering, a phonon distribution mismatch (differences in bulk phonon distributions due to differences in interfacial scattering rates[18]) may also give rise to an additional thermal boundary resistance. Han et al. 2023 found that a large thermal boundary resistance exists at the interface of Si/SiGe alloys despite the absence of interfacial scattering[18].After deriving the local distribution

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of interfacial phonons employing the Boltzmann transport equation and Monte Carlo methods, it was concluded that the imbalance of phonon distributions and the mismatch are responsible for the increased thermal boundary resistance, i.e., the difference in bulk phonon distributions due to the different scattering rates between the Si and SiGe alloys, which triggers additional entropy generation near the interface and significantly increases the thermal resistance[18].

In 2024, based on the previous study, Han et al. further investigated the Si/SiGe alloy interface and found that the thermal boundary resistance there increased rapidly with the concentration of germanium, which could be reduced by lowering the concentration of germanium[19]. The study of Han et al. provided a new direction as to whether thermal boundary resistances due to the mismatch of the non-equilibrium distributions of phonons exist at other interfaces as well, as well as a method for predicting and reducing the thermal boundary resistance. methods, and their findings undoubtedly provide certain new directions for future research development.

7. Conclusions and outlook

This study begins by introducing the Acoustic Mismatch Model (AMM) and Diffuse Mismatch Model (DMM), which predict thermal boundary resistance (TBR) under perfectly smooth and fully disordered interfaces, respectively.

To address arbitrary surface roughness, the Mixed Mismatch Model (MMM) is reviewed. Experimental validation shows that MMM accurately predicts TBR for interfaces with varying roughness.

Existing roughness-aware models focus on low-to-moderate temperatures, neglecting high-temperature regimes. This study highlights the dominant role of inelastic phonon scattering at elevated temperatures. The Joint Frequency Diffuse Mismatch Model (JFDMM) better predicts TBR by accounting for vibrational mode interactions, showing that TBR decreases with increasing temperature.

The Two-Temperature Model (TTM) demonstrates that electron-phonon coupling enhances thermal conductance by modifying phonon scattering rates and frequencies, reducing TBR.

Recent studies identify phonon distribution mismatch—due to differing interfacial scattering rates—as a key factor in Si/SiGe TBR. Increasing Ge concentration raises TBR, but reducing Ge content mitigates this effect.

Looking ahead, future research should prioritize the development of dynamic and coupled modeling approaches that integrate various factors affecting TBR. This includes combining the strengths of existing models like MMM and MHHIM to better predict TBR under varying conditions. Additionally, advanced experimental techniques are needed to validate and refine these theoretical models, ensuring their accuracy and applicability in real-world applications. Finally, enhancing our understanding of phonon transport in complex materials and interfaces will be crucial for improving thermal management in next-generation micro- and nanodevices.

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