Using the Callaway Model to Deduce Relevant Phonon Scattering Processes: The Importance of Phonon Dispersion

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The thermal conductivity $\kappa$ of a material is an important parameter in many different applications. Optimization strategies of $\kappa$ often require insight into the dominant phonon scattering processes of the material under study. The Callaway model is widely used as an experimentalist’s tool to analyze the lattice part of the thermal conductivity, $\kappa_l$. Here, we investigate how deviations from the implicitly assumed linear phonon dispersion relation affect $\kappa_l$ and in turn conclusions regarding the relevant phonon scattering processes. As an example, we show for the half-Heusler system (Hf,Zr,Ti)NiSn, that relying on the Callaway model in its simplest form has earlier resulted in a misinterpretation of experimental values by assigning the low measured $\kappa_l$ with unphysically strong phonon scattering in these materials. Instead, we propose an implementation of more realistic phonon dispersion curves, combined with empirical expressions for typical phonon scattering processes, which leads to far better quantitative agreement with both theoretical and experimental values. This method can easily be extended to other materials with known phonon dispersion relations.

1. Introduction

The thermal conductivity $\kappa$ is an important material property in many applications including for example heat management in integrated circuit design,[13] protective coatings,[14] and thermoelectrics.[15] $\kappa$ usually has contributions from electronic charge carriers, $\kappa_e$, and lattice vibrations, $\kappa_l$. For a given material, $\kappa_l$ can be modified by microstructural engineering and the control of phonon scattering centers, while $\kappa_e$ is rigidly connected to the electrical conductivity via the Wiedemann–Franz law. For applications, where both the thermal and electrical conductivity are important for the optimization of performance, only $\kappa_l$ can be independently optimized, and thus can become of prime importance for optimizing the thermal conductivity.[14,15] Deducing the relevant microscopic phonon scattering processes from the experimentally measured, macroscopic $\kappa_l$ is often challenging, but required in order to develop efficient strategies to optimize $\kappa_l$ for the given application.

Density functional theory (DFT) based ab initio methods scale unfavorably with the system size, due to the need for higher order perturbation terms, and therefore require high, cost-intensive computational power. Despite enormous progress during the last years,[6–15] these methods are still mainly used to describe specific, well defined material systems, so that fast, routine analysis of experimental data is not feasible at the moment. Therefore, experimental data is still often analyzed using simplified models developed decades ago.

A much used simplified model is the “Callaway model,” which is based on the Debye treatment of phonons and calculates the lattice thermal conductivity of a material via an effective phonon relaxation time $\tau$. In its common form, the Callaway model is implicitly assuming a linear $\omega(k)$ phonon dispersion throughout the 1st Brillouin zone (1.BZ). Under this assumption, the group velocity, $v_g = \omega/k$, is constant and identical to the phase velocity, $v_p = \omega/v_p$, and sound velocity, $v_s = \omega/dk$.

However, real materials all show deviations from the simple idealized dispersion, and the goal of the present paper is to demonstrate the errors introduced in the calculated lattice thermal conductivity by using the standard Callaway model. By implementing a simple phonon dispersion into the model, we show that it gives a significantly better agreement with results obtained by experimental and higher-level theoretical methods. This generalization can easily be extended to other material systems, to deduce the relevant phonon scattering processes from experimental data, without the computational cost of an ab initio based theoretical analysis.

2. Calculation of Thermal Conductivity

Within the limits of the relaxation time approximation and neglecting the small influence of N-processes at elevated temperatures, $\kappa_{l,i}$ of the i-th acoustic phonon mode is generally given as[18]

$$\kappa_{l,i} = \frac{1}{3} \int_0^{\omega_{\text{Max}}(k_i)} C_{V,i}(\omega) v_{g,i}(\omega) \tau(\omega) d\omega$$

(1)
where \( C_{v,Z}(\omega) \) is the spectral specific heat, \( \tau_i(\omega) \) the relaxation time, and \( v_{g,Z}(\omega) \) the group velocity of this mode. All phonons up to a maximum cut-off frequency \( \omega_{\text{max}} \) are considered in the integral. The total lattice thermal conductivity is then obtained as a sum over the contributions from the two transversal and one longitudinal acoustic modes. As many parameters entering the calculations are only found in the literature as an average over the three acoustic modes, we here use these average values instead to ease comparison with reported results. For example, the average sound velocity \( v_i \) is related to the velocity of the longitudinal, \( v_l \), and transversal modes, \( v_\perp \) via \( v_i = \left[ 1/3 \cdot v_l^{-3} + 2v_\perp^{-3} \right]^{1/3} \). Adding the contributions of the three acoustic phonon branches, using the Debye expression for the specific heat, and \( x = \hbar \omega/k_B T \), Equation (1) can be rewritten as:

\[
\kappa_i = \frac{k_B}{2\pi^2 v_i} \left( \frac{k_B T}{\hbar} \right)^3 \int_0^{\hbar \omega_{\text{max}}/v_i T} \tau(x) \frac{v_i(x)x^3 e^x}{v_p(x)^3 (e^x - 1)^2} \, dx
\]

When further assuming a linear dispersion, that is, \( v_\perp = v_p = v \), Equation (2) simplifies to the commonly used “Callaway expression”:

\[
\kappa_i = \frac{k_B}{2\pi^2 v} \left( \frac{k_B T}{\hbar} \right)^3 \int_0^{\hbar \omega_{\text{max}}/v T} \tau(x) \frac{x^4 e^x}{(e^x - 1)^2} \, dx
\]

As a model system, we choose here the half-Heusler XNiSn, \( X = \text{Hf, Zr, Ti} \), which has attracted considerable interest due to the combination of environmental abundance, non-toxicity, and promising thermoelectric properties. In order to decrease the high \( \kappa_i \) of these alloys, mass disorder on the X-site has been widely investigated. \( X \) et al. concluded on a dominating role of electron-phonon scattering in a wide phonon frequency range to describe the experimentally obtained \( \kappa_i \) of these materials. Their analysis was based on Equation (3) in combination with empirical expressions for the scattering times \( \tau_i \) of the individual scattering processes. However, the scattering rate for electron-phonon scattering should scale with the concentration of free electrons in the system. If electron-phonon scattering was a dominant contribution to the total \( \kappa_i \) of XNiSn, one should observe a significant reduction of \( \kappa_i \) with increasing charge carrier concentration. However, in systematic doping studies, \( \kappa_i \) shows no clear trend with varying carrier concentration. On the contrary, we have recently reported the good agreement of experimental values of \( \kappa_i \) for XNiSn and ab initio DFT calculations, without taking into account electron-phonon scattering. In the following, we will therefore use those reported DFT values as an experimentally confirmed reference for the analysis in the present paper.

In order to calculate the lattice thermal conductivity via Equation (2), one needs (a) a cut-off frequency \( \omega_{\text{max}} \) as an integration limit, (b) an expression for the specific form of the phonon dispersion relation \( \omega(k) \), and (c) an expression for the spectral phonon relaxation time \( \tau(\omega) \).

An obvious shortcoming of the frequently used Equation (3) is the implicitly assumed linear phonon dispersion throughout the 1. BZ. This was originally justified, as Callaway’s model was intended to describe \( \kappa_i \) at low temperatures, where most phonons populate states in the linear regime of the dispersion curves around the center of the 1.BZ, \( \Gamma \). However, at elevated temperatures, also phonon modes outside the linear regime of the dispersion relation contribute to the thermal conduction. Estimating the integration cut-off by extrapolating the linear region of the phonon dispersion curves to the boundary of the 1. BZ will thus generally result in too high \( \omega_{\text{max}} \) and thus too high \( \kappa_i \). Instead, it was suggested to use the phonon frequency at the zone boundary as a cut-off in Equation (3), which can be obtained by, for example, inelastic neutron diffraction experiments or computational studies.

As a second requirement to calculate \( \kappa_i \) by Equation (2), one has to assume a certain shape of the phonon dispersion relation, providing expressions for \( v_p(x) \) and \( v_p(x) \). Here, we calculate \( \kappa_i \) by three different methods, schematically shown in Figure 1(a):

(i) The “Debye cut-off” model, that is, using linear phonon dispersion throughout the Brillouin zone, with \( v_p = v_p = v_i = v \).

(ii) The “Phonon DOS cut-off” model: As in (i), but limiting the integral in Equation (3) to frequencies below the phonon frequency at the Brillouin zone boundary, \( \omega_{\text{max}} \), as obtained from computational phonon dispersion curves. Note that this approach still assumes the identity of sound, group, and phase velocity for all phonon modes considered in the integral.

(iii) The “Phonon dispersion” model, which approximates the average phonon dispersion by a simple polynomial, \( \omega(k) = a \cdot k^l + b \cdot k^i + c \cdot k \). The coefficients \( a \) and \( b \) for the different compositions XNiSn are obtained from the condition \( \omega(k = k_{\text{max}}) = \omega_{\text{max}} \) and \( \omega(k = 0) = \omega_{\text{max}} \). From the approximated \( \omega(k) \), the frequency dependent \( v_p(\omega) \) and \( v_p(\omega) \) in Equation (2) can be easily obtained.

Lastly, in order to calculate the thermal conductivity for the three different models using Equation (2), information on the frequency dependent relaxation time \( \tau(\omega) \) is needed. According to Matthiessen’s rule, the total relaxation time \( \tau(\omega) \) is related to the relaxation time \( \tau_i(\omega) \) of the \( i \)-th scattering process via \( \tau(\omega)^{-1} = \sum_i \tau_i(\omega)^{-1} \). In the present calculation, we consider three different phonon scattering mechanisms: Umklapp, mass disorder, and grain boundary scattering. Importantly, this is the same set of phonon relaxation processes contributing to the total relaxation time \( \tau \) as used in earlier DFT calculations with good agreement with experimental values. For the relaxation times of the different processes, we adopt commonly used empirical expressions, summarized in Table 1. There, \( \gamma, \theta_{\text{max}} = \hbar \omega_{\text{max}}/k_B T, \omega, \gamma, \theta_{\text{max}} \) are, respectively, the Grüneisen parameter, the frequency cut-off, the average grain size, the average atomic mass on the X-sublattice, the average mass of all atoms, the relative concentration of Hf, Zr, or Ti, and their atomic mass. \( \gamma \) is related to the anharmonicity of the chemical bonds of the structure. Reported values of \( \gamma \) for XNiSn vary in the range from 0.8 to 2 depending on the employed method, but do not show a significant variation with X when using the same methodology. Here, we use \( \gamma = 2 \) for all compositions, but our results are not very dependent on this particular choice. For point-defect scattering, we also neglect the...
Figure 1. a) Schematic of the three different approximations to the Callaway model used here, as explained in the text. b) Phonon dispersion for TiNiSn along selected high symmetry directions as calculated by DFT. Optical modes are grayed out for clarity. The linear extrapolation around \( \Gamma \) leads to a significant overestimation of cut-off frequencies for both longitudinal (LA) and transversal acoustic (TA) phonon branches.

3. Results and Discussion

From the available DFT-based phonon dispersion curves, Figure 1(b), for the three unmixed compounds, \((X = \text{Hf}, \text{Zr}, \text{Ti})\)\(^{35,46}\) we obtained the sound velocity \(v_s\) from a linear fit around the \( \Gamma \)-point, as shown in Table 2. From the calculated dispersion curves, we can then quantify the overestimation of the cut-off frequency in Equation (2), when erroneously using the linear phonon dispersion throughout the 1.BZ, instead of the real phonon frequency at the zone boundary. Extrapolating the linear region of all phonon branches of TiNiSn leads to much higher phonon frequencies at the Brillouin zone boundary, \(\omega_{\text{Debye}}\), than the frequencies obtained by DFT. This is most pronounced for the LA branch, but also extrapolating the TA branches results in an overestimation of the maximum frequency of around 40%. Averaging over the three acoustic phonon branches and the different \( k \)-space directions, the average frequency at the zone boundary is \(\omega_{\text{Max}} \approx 0.6 \omega_{\text{Debye}}\), fairly independent of the composition \(X\), cf. Table 2.

**Table 1.** Expressions for the relaxation rates of the different scattering processes considered here.

| Scattering process | Scattering rate | Reference |
|--------------------|-----------------|-----------|
| Umklapp            | \(\tau_{\text{U}}^{-1}(\omega) = \frac{4\pi\hbar^2}{M_{\text{eq}}\omega^6} \exp\left(-\frac{\sqrt{3}k_D^6}{\hbar\omega}\right) \times \omega^2\) | \([42,43,44]\) |
| Point defect       | \(\tau_{\text{PD}}^{-1}(\omega) = \frac{k_D^6}{12\pi V_F(T_0)^4} \left(\frac{T_0}{T_F}\right)^5 \sum_{\text{Hf}} \sum_{\text{Zr}} \sum_{\text{Ti}} C_i \left(m_i - \frac{m}{2}\right)^\gamma \times \omega^4\) | \([41,42,44]\) |
| Grain boundary     | \(\tau_{\text{GB}}^{-1}(\omega) = \frac{v_p(\omega)}{d}\) | \([45]\) |

Symbol explanation and further information is given in the text.
those materials, we emphasize that one a priori cannot simply express the contribution of the optical modes like in Equation (1) and add them to the acoustic $\kappa_l$. The empirical scattering rates $\tau/C_0$, as summarized in Table 1, have been developed only taking into account acoustic modes, so that some influence of the optical branches, like scattering from or into these modes, might effectively already be incorporated in the expression of $\tau/C_0$. For $X$ NiSn, the contribution of optical modes to the total $\kappa_l$ as obtained from the full dispersion DFT calculation is below 10%, Figure 3, that is, below typical accuracies of a Callaway-type analysis.

Table 2. The longitudinal $\nu_l$, transversal $\nu_t$, average sound velocity $\nu_v$, Debye cut-off $\omega_{Dyeb}^\text{Dyeb}$, and phonon DOS cut-off $\omega_{Dyeb}^\text{Max}$ for the three unmixed compounds.

|     | $\nu_l$ [m/s] | $\nu_t$ [m/s] | $\nu_v$ [m/s] | $\omega_{Dyeb}^\text{Dyeb}$ [THz] | $\omega_{Dyeb}^\text{Max}$ [THz] |
|-----|---------------|---------------|---------------|-----------------------------------|----------------------------------|
| Ti  | 2991          | 5513          | 3337          | 50.3                              | 30.0                             |
| Zr  | 2878          | 5437          | 3217          | 47.0                              | 30.6                             |
| Hf  | 2575          | 4793          | 2875          | 42.2                              | 27.4                             |

Values for the mixed compositions are obtained by linear interpolation of the unmixed values. There is a good agreement with experimental values obtained for samples of similar composition (±5%).

Our results emphasize that the linear dispersion relation as assumed in Equation (3) predicts a $\kappa_l$ which is much larger than values typically measured experimentally. To make values of $\kappa_l$ calculated by the Debye–Callaway model similar to experimental ones, different approaches have been reported in the literature. These include introducing additional phonon relaxation processes, such as electron-phonon scattering, reducing the effective relaxation time for low and medium frequency phonons, or using an empirical expression for $\tau^{-1} = A\omega^4 + B\omega^2 + v/d$, with $A$, $B$, and $d$ being adjustable parameters. In the latter approach, determining $A$, $B$, and $d$ may well reproduce the experimentally measured $\kappa_l$, but the physical meaning of these parameters can be unclear. More severely, adding additional phonon scattering processes to the analysis changes the physical interpretation of the obtained results.

In addition, both these modifications only target the integrated $\kappa_l$, while the spectral $\partial \kappa(\omega)/\partial \omega$ would show finite values up to the Debye cut-off $\omega_{Dyeb}^\text{Dyeb}$, in disagreement with physical intuition and DFT results. As we show here, much better agreement for both $\kappa_l$ (Figure 2) and $\partial \kappa(\omega)/\partial \omega$ (Figure 3) is obtained when taking into account the dispersive nature of...
phonons, without changing the type or strength of the dominant scattering mechanisms. In particular, the simple model phonon dispersion as used here in combination with the empirical expressions for the different scattering processes, but without any further fitting parameter, reproduces the cost-intensive DFT results both on a microscopic and macroscopic level. We chose a third-order polynomial to mimic a more realistic phonon dispersion. Analytical functions or discrete parametrizations with more free parameters may describe the actual phonon dispersion curves even better and may change the calculated $\kappa_l$ somewhat. One should, however, bear in mind that also the relaxation times for the different scattering processes given in Table 1 are based on simple, empirical expressions, so that further refinement of the phonon dispersion without modification of the phonon scattering may quickly cross the limits of the chosen model.

Finally, we note that both the improved models (ii) and (iii) require phonon dispersion curves of the material under study. The experimental determination of these dispersion curves can be challenging, due to required sample dimensions and limited access to scattering facilities, while computational methods nowadays routinely provide reliable data. As compared to first principle calculations of thermal transport properties, the phonon dispersion curves required for model (ii) and (iii) are computationally much less demanding, as only harmonic terms have to be considered.\[5\]

4. Conclusion

We conclude that the Callaway model with implementation of the effects of phonon dispersion is a simple but useful model to analyze the lattice thermal conductivity $\kappa_l$ of a material. In contrast, the Callaway model in the often used simplification of Equation (3) is generally too simple to deduce the dominant phonon scattering processes at elevated temperatures, and can result in misleading strategies to optimize $\kappa_l$. We have shown, that combining a simple polynomial phonon dispersion relation and empirical expressions for relevant scattering processes without any adjustable parameters reproduces $\kappa_l$ of a (Hf,Zr,Ti)NiSn model system both qualitatively and quantitatively. This model can easily be extended to understand $\kappa_l$ of a wide range of other material systems, as long as information on the phonon dispersion is available.

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Conflict of Interest

The authors declare no conflict of interest.

Keywords

Callaway model, phonon scattering, thermal conductivity

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