Models for the electronic transport properties of thermoelectric materials

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1 Introduction

Providing the world with sustainable energy is one of the more challenging problems of modern society. While the world's hunger for power increases the supply of fossil fuel is decreasing. Sustainable energy sources like solar and wind power are providing us with solutions, but a large amount of waste heat is dumped while it can be used to generate energy through thermoelectric devices.

These thermoelectric devices can convert a heat flow directly into energy. The materials of which such a device is made are solid and the device is without moving parts. Therefore they are reliable, silent and can be relatively small. Although there efficiency is not very good, these properties allows them to be used in several locations.

Furthermore, the process of generating energy from heat can also be reversed. Thus by applying energy the material can transport heat, which can be used for cooling purposes.

While developing the theory behind this in the fifties, bismuth telluride was found as a relatively efficient material. After commercializing it there was little research and improvement on better materials. This lasted until the beginning of the nineties, when new directions for improvement were discovered.

One of these directions is the use of nano inclusions. These are nano scale particles that are embedded into a host thermoelectric material. The effect of these inclusions is that the conduction of heat is reduced while the electrical power generation is improved. Overall this improves the efficiency of the material. Furthermore, by giving more parameters, like particle size, the material can be tuned to function optimally at the operating conditions.

Modelling the effect of these nano inclusions is essential. Without it the search for good combinations of materials for both the host and the inclusion is like playing roulette. With models the effect of including particles, their size and other parameters can be estimated and better searching is possible. Furthermore, ideas for improving the materials might come from a better understanding gained through these models.

This report looks into the current model being used for simulating the electrical part of thermoelectric materials. In addition it makes an overview over the relevant parameters for choosing a model for nano inclusions. Followed by an outline of the steps needed to implement the model as a simulation. With an conclusion and outlook on further steps needed as last part.

2 Model

Presenting the model for a material with nano inclusions can be decomposed into several parts. The first part is an introduction into the thermoelectric effect. Followed by a treatment of the model that is used for the past decades to model bulk material. After discussing the validity of the model the extension to nanoinclusions is made.

2.1 Basic thermo electrics

There are several thermoelectric effects. The two most important ones are the Seebeck and Peltier effect. The Seebeck effect is the creation of a potential difference when a metal or semiconductor has a thermal gradient. The Peltier effect is that a current flowing through a junction cools or heats it (depending on the junction and direction of flow). Both effects are caused by the charge carriers in the material both providing an electrical and energy (heat) current. For energy generating the Seebeck effect is the most interesting one, as one can use the difference in potential to create a power source. [1]

The Seebeck effect is caused by the diffusion of charge carriers in metals or semiconductors. The charge carriers on the hot side of the material have higher speeds than those on the cooler

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[1] Note though it requires more than one material, as connecting wire to a single material would also create the same effect across the connection wires. Which would practically cancel the effect.

side. The result is that the carriers diffuse to the cool side of the material. This carrier buildup on the cool side causes an electric field which counteracts the diffusion force.

The strength of this effect can be described by the Seebeck coefficient

$$S = -\frac{\Delta V}{\Delta T}. \tag{1}$$

Where V is the potential difference which is generated by the temperature difference T. For most metals the Seebeck coefficient is on the order of a few μV/K, while for sufficiently doped semiconductors it will on the order of several 100 μK/V. The sign of the S depends on the relative direction of the potential difference to the temperature gradient. Roughly speaking in materials where electrons dominate the transport the sign is negative while when holes dominate transport the sign is positive.

Though a good Seebeck coefficient is essential for a thermoelectric material, it is not the only parameter in its efficiency. For that there is the figure of merit

$$ZT = \frac{S^2 \sigma T}{\kappa_p + \kappa_e}. \tag{2}$$

Where σ is the electrical conductivity, κ_p and κ_e are the thermal conductivity of the lattice (phonons) and the charge carriers and T is the temperature at which these are measured. The figure of merit is directly related to the efficiency of a thermoelectric device, thus larger ZT are better.

The basic approaches to improving ZT are to optimize the power factor $S^2\sigma$ and to reduce the thermal conductivity of the lattice κ_p to the same level as κ_e [1]. Thus the problem of improving the efficiency is the same as finding a material with a higher ZT.

2.2 Single band

The problem with ZT is that the separate parameters still need to be calculated. The model of choice, for many years, for this problem is the Boltzmann equation with relaxation time approximation. Which is a statistical model for particle diffusion in non equilibrium situations.

The basic idea behind this model is to treat the non equilibrium situation as a disturbance of the equilibrium version. In equilibrium the energy bands of the material are filled according to the Fermi-Dirac distribution

$$f(E) = \left(e^{\frac{E-\mu}{k_b T}} + 1\right)^{-1}. \tag{3}$$

With E the energy, μ the Fermi level, T the absolute temperature and k_b the Boltzmann constant. The difference from equilibrium causes forces on the particles resulting in a shift in the distribution, described by the Boltzmann equation. Though the particles also collide with each other and possible other things. Under the relaxation time approximation this is modeled with a relaxation time $\tau(E)$, denoting the average time between collisions for a particle at energy E.

Furthermore assuming that the difference between the equilibrium situation and the perturbed non equilibrium is small, a result can be derived for S, σ and κ_e. Assuming there is only a single energy band and the material is isotropic (S and other values are direction independent), the resulting formulas are for S and σ are given by [5]

$$\begin{aligned} \sigma &= \frac{2q^2}{3m^*} \int_0^\infty \tau(E) g(E) E \left(-\frac{\partial f}{\partial E}\right) \mathrm{d}E, & (4) \\ S &= \frac{1}{qT} \left[\frac{\int_0^\infty \tau(E) g(E) E (E-\mu) \left(-\frac{\partial f}{\partial E}\right) \mathrm{d}E}{\int_0^\infty \tau(E) g(E) E \left(-\frac{\partial f}{\partial E}\right) \mathrm{d}E} \right]. & (5) \end{aligned}$$

The charge carrier charge q and its effective mass m^* are input parameters. Thus there are three unknown quantities in these equations, the relaxation time $\tau(E)$ of a charge carrier and the density of states $g(E)$ (DOS) of the band and, hidden in f, the Fermi level μ. Where the reference point for E and μ is the band edge.

Note, the previous formulas slightly vary from paper to paper. In several papers (e.g. [3]) and [6]) the factor E in the integral is replaced with v^2, the electron group velocity squared, with possibly an extra constant. Though [5] suggests that $v = \sqrt{\frac{2E}{m^*}}$, which would explain the difference. Other papers, like [2] and [9], replace it with an extra correcting factor, probably correcting for the different group velocity, when taking into account the DOS. The choice to use E instead of, assumed to be more correct, v^2 was to keep things simple for a first implementation. In addition the formula for κ_e is left out as there is no paper that states it with the DOS, a bit of puzzeling with the formulas suggests

$$\kappa_e \overset{?}{=} \frac{2}{3Tm^*}\left(\int_0^\infty \tau(E)g(E)E^3\left(-\frac{\partial f}{\partial E}\right)\mathrm{d}E - \frac{\left(\int_0^\infty \tau(E)g(E)E^2\left(-\frac{\partial f}{\partial E}\right)\mathrm{d}E\right)^2}{\int_0^\infty \tau(E)g(E)E\left(-\frac{\partial f}{\partial E}\right)\mathrm{d}E}\right). \tag{6}$$

Though before using this formula it should be looked up.

2.3 Extending to multiple bands

Though the semiconductors are heavily doped, modelling it as a single band is not fully realistic. The extension to multiple bands is quite easy by using

$$\begin{aligned} \sigma &= \sum_i \sigma_i \text{ and} \\ S &= \frac{\sum_i S_i\sigma_i}{\sum_i \sigma_i}. \end{aligned}$$

Where S_i and σ_i are the contributions from each band, calculated by using (4) and (5). Though this addition seems trivial and a logical result from expanding $g(E)$ to more bands, a note of caution is in place. For all the formulas, like those for $\tau(E)$, σ and S, the reference energy, $E = 0$, is taking to be the top (valence) or bottom (conduction) of the band, with the energy going up when going higher or deeper in the band. To correct for this two steps need to be taken. The Fermi level must be adjusted to match the reference energy of the band. Secondly, when the energy (of the carrier) increases (larger E) when integrating over a valence band, the absolute energy level decreases. To compensate for this $f(E)$ and $\frac{\partial f}{\partial E}(E)$ should be replaced with $f(-E)$ and $\frac{\partial f}{\partial E}(-E)$.

2.4 Fermi level

The first unknown parameter is the Fermi level μ. Which is related to the doping level, and thus the charge carrier density n. For a single band model the Fermi level is the solution of

$$n = \int_0^\infty g(E)f(E)\,\mathrm{d}E = \int_0^\infty g(E)\left(e^{\frac{E-\mu}{k_bT}}+1\right)^{-1}\mathrm{d}E. \tag{7}$$

For a model with multiple bands this gets a bit more complicated. The problem is that there is a need to deal with both holes and electrons, following [8] the doping level n_d can be defined as the absolute difference between the concentration of holes and electrons. Thus using $n_{e,i}$ as the concentration of electrons in conduction band i and $n_{h,i}$ for the hole concentration in valence band i, then n_d can be expressed as

$$n_d = \left|\sum_i n_{h,i} - \sum_i n_{e,i}\right|. \tag{8}$$

Where $n_{e,i}$ and n_{h_i} can be calculated by (7). The note about correcting for energy levels when extending to multiple bands also applies here. [2]

The absolute value is taken as both holes and electrons can dominate. Though this ensures a positive n_d, it raises the problem that this also causes the equation to have two solutions for μ, one near the conduction bands (with excess holes) and one near the valence bands (with excess electrons). The correct one depending on the type of dopant. For a computation of μ this is not practical and a better option would be to remove the absolute value. When doing so the doping concentration should also reflect the type of dopant, where n-type dopants use negative concentrations (as they add electrons).

2.5 Density of states

The second open question was what the density of states is, which follows from the dispersion relation. The standard model for the energy dispersion relation is the Kane model [2, 5]

$$\frac{\hbar^2}{2}\left(\frac{k_l^2}{m_l^*}+\frac{2k_t^2}{m_t^*}\right)=E+\alpha E^2. \tag{9}$$

Where $k_{l,t}$ are the wave vectors and $m^*_{l,t}$ the effective masses in the longitudinal and transverse direction. Which corrects for the not perfectly parabolic form of the energy bands using the extra parameter α. For small band gap semiconductors $\alpha = 1/E_g$ is a good approximation, with E_g is the band gap [5]. (Note: most papers directly plug in the relation for α)

From this dispersion relation the density of state follows [5]

$$g(E)=\frac{\sqrt{2}}{\pi^2}\left(\frac{m^*}{\hbar^2}\right)^{3/2}\sqrt{E(1+E/E_g)}(1+2E/E_g). \tag{10}$$

Where the effective mass $m^* = (\beta^2 m_l^* m_t^{*2})^{1/3}$, with β being the degeneracy if the Fermi surfaces. Note that this also eliminates the separate effective masses for longitudinal and transverse directions, making the model isotropic.

2.6 Relaxation time

The last open question for using (4) and (5) is the relaxation time.. The relaxation time is used to model several scattering processes inside the material. In general the scattering events are assumed to be independent and random. Furthermore they should be elastic scattering for the relaxation time approximation to hold. Making these assumption the scattering processes can be treated separately and combined using Matthiessen's rule [8]

$$\tau^{-1}=\sum \tau_i^{-1}. \tag{11}$$

Where each τ_i is the relaxation time for a specific scattering source.

Then the question can be restated as what scattering sources are there and what are their relaxation times. The answer on the first question depends on the material that is modeled. The second question is a bit harder as there are, for each scattering mechanism, several relaxation times in literature, but according to [3] they give similar results.

Though most expressions for the relaxation times of a specific scattering mechanism differ they are quite similar. Most of the relaxation times can roughly be fitted to the form

$$\tau(E)=aE^s h(E). \tag{12}$$

Where s is the general energy dependence, a is a constant denoting the strength of the scattering and h is a unitless function. When comparing two different expressions for a relaxation time the

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[2] In [8] formula (5) they have expanded (8) and filled in their DOS. The result is a formula spanning over more than two lines and therefore the subtle difference between conduction and valence bands are easily lost. Which is also a reason for keeping this step abstracted away.

difference is (most of the time) in the correction function h, which normally is of about unit size. The value of s, the general energy dependence, is more important and is a characterizing aspect of the scattering mechanism.

For most of the papers on these simulations take three or four scattering processes into account. Two or three scattering rates are used to model interaction with phonons and a last scattering rate for ionized impurity scattering. The interaction with phonons is split up between non polar optical phonon scattering and deformation potential scattering[3] on both acoustic and optical phonons.

A quite simple model for these scattering modes is used by [5]. This model will the examples to discus some intricacies of the scattering rates.

Starting with the relatively simple polar optical phonon scattering (only present in polar materials),

$$\tau_{o-ph}(E) = E^{1/2} \frac{h^2}{\sqrt{2m^*} e^2 k_B T \left(\varepsilon_\infty^{-1} - \varepsilon_0^{-1}\right)}. \tag{13}$$

with ε_∞ the high frequency dielectric constant and ε_0 the static dielectric constant. This fits nicely on the general form for relaxation times with $s = \frac{1}{2}$, $h(E) = 1$ with the fraction being the constant a. It is also one of the most convenient relaxation times to work with as all parameters can be measured.

The second scattering process considered is the deformation potential scattering. Only the deformation potential from acoustic phonons is included using,

$$\tau_{a-ph}(E) = E^{-1/2} \frac{h^4}{8\pi^3} \frac{\rho v_L^2}{k_B T} \frac{1}{(2m^*)^{3/2} D^2}. \tag{14}$$

Where ρ is the density of the material, v_L is the longitudinal speed of sound and D is the deformation potential constant. The deformation potential constant is an empirical parameter and needs to be fitted with usual values in the range of $5 - 15$ eV. Similar expressions also exist for deformation potential scattering on optical phonons, normally with the same temperature and energy dependence. Therefore when there is no good model for one of the scattering modes, like in [3], one relation is used to model both acoustic and optical phonon deformation potential scattering.[4]

The last scattering mode to include is the scattering on ionized impurities. The expression used for the relaxation time is

$$\tau_{imp}(E) = E^{3/2} \left[\frac{Z^2 e^4 N_i}{16\pi\sqrt{2m^*}\varepsilon} \ln\left(1 + \left(\frac{2E}{E_m}\right)^2\right)\right]^{-1} \tag{15}$$

With Z the charge of an impurity, N_i the concentration, ε the dielectric constant of the material. Furthermore $E_m = \frac{Ze^2}{4\pi\varepsilon r_m}$ is the potential energy at a distance r_m from an impurity, with r_m taken to be half the distance between impurities. This is quite a simple model for impurity scattering, most of the models also include some form of screening.

2.7 Limits of the model

The model presented has quite some limits. Most papers discussing these equations and their modifications for nano inclusions only compare the results from their calculations with experimental findings or reference values, and from the good fit assume that it is valid.

One notable exception is [3], which has some notes on the validity of using the Boltzmann equation for highly doped thermoelectric materials. A problem is the applicability of the Boltzmann equation, which is a model for particles, thus discarding any wave effects like interference. To be valid it is necessary for the mean free path of an electron to be much larger than its wavelength. In their paper this was not the case with the bulk of the electrons in fact having a mean free

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[3] This effect is caused by the phonons, which are lattice vibrations. The vibrations cause deformations in the potential on which carriers can scatter.

[4] A probable reason is that they are interchangeable when fitting due to the same energy and temperature dependence.

path smaller than their wavelength. They note that a possible cause might be that it is caused by inaccurate scattering models. These are derived for low doping concentrations, while they were used in a case with a heavily doped material, thus they might overestimate the scattering rates.

But the very short mean free path might be a problem of their situation. Their model and calculations are targeted at SiGe nano composite, fitting part of their parameters used for one relaxation time. Even though their discussion highlights the two major problems of the model. Both the particle approach based on the Boltzmann equation nor the use in highly doped materials might be valid.

A second problem might be in the validity of the relaxation time approximation, which requires that the scattering mechanism is elastic. This is not the case for non polar optical phonon scattering. But as noted in [3], non polar optical phonons have relatively low energy ($20-50$meV) which is low compared to the Fermi level which is inside their band by up to 0.2eV in their study. Therefor they assume that elastic collisions are a good approximation. Also [8] use this assumption, but without further motivation.

The question remains whether or not this assumption is reasonable. There are some positive points for taking the assumption. First of all, these models have worked for the past decades, though the question is how close they were. Secondly, a high doping level is needed in thermoelectric materials, otherwise the minority charge carriers will greatly reduce S. Therefore the energy of an average charge carrier will be relatively high. Though there is a negative point, the non polar optical phonon scattering is, assuming it is elastic, according to the approximations the dominant scattering mechanisms at low energy. As it stands it seems that it is best to assume elastic scattering.

2.8 Adding nano inclusions

Now that the basic model for the electrical properties of semiconductors has been described, the target of adding nano inclusions can be modeled. For this it is first needed to get an idea of the effect of the nano inclusions on the material. Followed by several steps needed lead to a good model for the inclusions.

The effects

When adding nano inclusions to a material so called 'bound charges' are formed. These are charge carriers that accumulate at the interface of the two materials, which is caused by the band bending. These bound carriers have two effects on the electrical properties of the material.

The first and most important one is that the bulk carriers scatter of the formed potential locally formed by the bound charges. The scattering probability for this effect is energy dependent and it mainly affects carriers with low energy. The result is that the conductivity σ decreases due to more scattering. Though the average excess energy of a carrier, $E-\mu$, increases. When this effect is balanced out correctly the power factor, $S^2\sigma$ of the figure of merit will increase. This technique of decreasing the number of low energy charge carriers is known as energy filtering[1].

The second effect is that the bound charges can form energy bands. This effect that is most interesting in combination with low dimensional inclusions (e.g. nano size dots). The regular potential differences formed by a lattice of these inclusions forms extra bands that contribute to the electronic properties. The nice property of these extra bands is that they can be tuned by adjusting the inclusions, and can thus be used to optimize the figure of merit.

Apart from the changes in electrical properties it also changes the phonon dynamics of the material. Although not the focus of this report this needs to be mentioned, as it is of great effect. Without the inclusions the phonon thermal conductivity κ_p is far greater than the electrical one (κ_e). But adding of the nano inclusions also causes extra scattering of interfaces for the phonons, with the effect that κ_p decreases. It can even be brought back to be comparable to κ_e [1].

Modeling the inclusions

The effects of the inclusion on the thermoelectric properties need to be added to the model. Both effects must be modeled separately as they have quite different effect on the model.

The second effect, the formation of extra bands, will not be treated in great depth as it requires very specific nano materials. The simple way of modeling these is to calculate the extra band(s) created by the structure of nano inclusions (see [9]). The electronic properties of the material are then calculated and added as with any other band.

The first effect, scattering of the bound charges, is modeled by adding an extra relaxation time. But for this to be valid in the standard model there are some requirements. As the model treats the material as bulk the inclusions should be distributed uniformly through the material. Secondly, as the charge carriers are modeled as particles the scattering of several things, including the inclusions or its interface. Therefore, no wavelike effects, like interference, should occur between two separate scattering events. [5] The last requirement is that the scattering is elastic and independent of any other scattering mechanism, when noted this is usually left as an assumption[7].

Calculating the relaxation time

The question remains then how the relaxation time should be calculated. For this it is needed to distinguish several cases.

The first factor is the volume density or fraction of the inclusions. For a small fraction of the inclusion material the basic properties of the host material (like the effective mass m^*) are not effected. For larger fractions the mixing properties are starting to deform these properties and these effects should thus be taken into account.

The second factor is the distance between the particles. When the distance is large enough (more than the mean free path), each particle can be treated as a separate scattering source. For smaller distances the effects of the particles start to overlap, one possibility is to use an effective medium approach.

The third factor is the size of the particle itself. Here the size as the length of the path that a carrier would travel inside the inclusion. If the particle is small relative to the mean free path of the carrier then it scatters of the whole particle. When the particle is large compared to the mean free path it will only see a small piece of the interface, and thus scatters of the interface.

Also important is the geometry and material of the inclusion. For simplicity most papers assume spherical inclusions, or take an abstract parameter like the amount of surface area per volume. While the material used is up to the specific case that is modeled.

To get to these properties several papers were studied, each taking a different material to investigate.

First of all there is [2], improved by [6], which models small low density metal inclusions. The approach is to numerically calculate the potential (using poisons equation) around the inclusion and use the Born approximation to calculate the scattering rate. For scattering the particle is seen as a single scattering target, which is needed for the small (few nm) particles they are using.

It's predecessor [3] is also quite interesting. It modeled SiGe nano composite, with large grains and interpolated material constants. They argue that as the particles are large only a small part of the interface is seen by the carrier. Thus the scattering rate can be calculated from the scattering of a small piece of the interface. Though unlike the previous paper they make an assumption about potential near the interface and then use the born-approximation. While the method is a worse (or older), the paper does contain quite a discussion on the validity of the approach used.

A combination of the previous two is [8], which studies nano composites in more general. It combines the numerically calculated potential with the scattering of interfaces. They focus primarily on using the calculated scattering probability to calculate the relaxation time, where the properties of both materials are taken into account.

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[5] Possible interference **might** be allowed when the distance is much larger than the mean free path ($\lambda = v\tau$). But then the effect of the inclusions is low, and can probably be neglected.

For higher concentration of particles [7] is interesting, introducing an effective medium approach to simulate the rest of the material around a particle.

3 Implementation

The model described in the previous chapter can be used for simulating thermoelectric materials. In this chapter the outline of such a simulation is described and possible ways for validation are discussed.

The first step for a simulation is to tune the model to the specific material. This choice is needed to use the right parameters, energy bands and scattering mechanisms.

The real simulation can then be build, which consists of the following steps:

1. Calculate the Fermi level μ for the given parameters, this is done by solving 7. This can be done by simple root finding algorithms.

2. Using the found value of μ the integrals for S and σ for each band can be calculated.

3. The total S and σ can be added up to form the final result.

While this seems to be a simple scheme there are some troubling points in it.

The most obvious problem is that all the integrals are indefinite, extending to infinite energy. Though most of the energy spectrum effectively doesn't contribute to the final value, as $f(E)$ and $\frac{\partial f}{\partial E}$ go rapidly to 0 when the energy increases. Thus limiting the integration to an upper bound can be justified. But then the question remains what this upper bound should be.

A fixed upper bound is does not work correctly, as the relevant part of the integral can strongly depend on the used parameters like T and μ. Thus a (validated) guess should be made at an appropriate upper bound dependent on these parameters.

To make a good guess it is best to look at the integral. The general form is that it starts at 0 for $E = 0$, increases to a maximum value at some E_{max} and then rapidly decreases due to the factor $f(E)$ or $\frac{\partial f}{\partial E}$. A reasonable upper bound could be a multiple of E_{max}, say ten times. This would make sure that an adaptive integration method, like MATLAB's `quad`, will detect the maximum, while not wasting accuracy and computing time on the negligible tail.

The second complicating point is the large dependence on T of the integrals for S and σ. Roughly speaking, when the temperature increases the maximum value decreases while the relevant width increases. In combination with a fixed absolute integration precision, as used by MATLAB's `quad`, this will result in bad accuracy, due to the varying magnitude of the integral. One solution is to switch from E to a dimensionless energy $\frac{E}{k_b T}$, normally called η. The use of η instead of E is common in papers and not really introduced nor motivated.

The third possible complicating point is caused by the relaxation times. The presented formulas in 2.6 are easy to compute for a specific energy. Though for some other relaxation times, especially for those from inclusions, this calculations becomes relatively expensive. When this is the case steps should probably be taken to prevent the integration of S and σ taking too much time.

3.1 Verification and validation

The simulation needs to be verified to work and possible assumptions need to be validated. For this several steps can be taken, which will be described here.

The primary goal for verification is to compare a simulation with values from literature. The best approach for this is to simulate bulk material (thus no inclusions) and compare the resulting values to the reference values. Good agreement shows that both the chosen (or fitted) parameters of the scattering rates and the included scattering rates are a good approximation.

Though the previous test sounds simple, just calculate and compare, it is the most difficult to get right. It tests only the correct result of the full simulation without testing subparts, thus the location of a possible flaw cannot be detected. For this it is better to look at the subparts, like the relaxation times, and see if changing variables (e.g. T) have the right effect on them.

Two notable exceptions are the Fermi level and the relaxation times. The Fermi level can probably be checked against literature values, especially if using a common semiconductor. This is quite important to get right as S and σ quite heavily depend on μ. The relaxation times can be compared to each other, each of them should be of about the same size. While not needed to be exactly of the same size, it is also not expected that one of the relaxation times is dominating the others.

When adding inclusions there is only one test, the comparison with experiments. This can be used to validate that the model of the inclusion scattering is correct.

3.2 Notes after own experimentation

A small test simulation was written based on [5]. Which was chosen as it seemed to be the simplest model, assuming only a single band and using simple scattering relations. While the results from the paper were not reproduced some lessons were learned from it.

The most important one is to check each formula for dimensions. While easy to check the result of not doing so is that hours can be wasted on finding the root cause of the incorrect value.

The second lesson is to always manually set the tolerance levels of algorithms. While MATLAB functions do have default tolerances they are probably not correct.

The third and last lesson was on single band models. While they look good as a first approximation for highly doped materials they have one big disadvantage. The behavior at higher temperatures is flawed, as they ignore the increasing (parasitic) contribution of the minority charge carriers. Thus a decrease in Seebeck coefficient at higher temperature can thus not be seen. As this is caused by both electrons and holes contributing to the Seebeck coefficient, but with opposite signs.

4 Conclusion and outlook

Several small steps have been set on the road to making a simulation for thermoelectric materials. The general model for semiconductor conductivity based on the Boltzmann equation with relaxation time approximation has been described. Furthermore several general parameters for nano inclusions are defined, like the particle size. With the effects of these parameters on the modelling being described. Several papers are categorised using these parameters to illustrate the effect on the models used for inclussion scattering.

In addition an outline of a simulation using the model is given. Which can be used to simulate a thermoelectric material both with and without inclusions. Of this simulation several points of attention are discussed with possible ways to handle them. Part of these the result of a, failed, first try at creating such a simulation.

For further work on this path to a simulation of a material with nanoinclusions several steps need to be made. First of all a choice of the host material needs to be made. For this material the appropriate scattering mechanisms with their relaxation times need to be found in literature or approximated. The second step is to identify the type of inclusions to use. Based on this decision a model can be chosen to use for calculating relaxation times.

For the calculation of the figure of merit ZT, only one parameter extra is needed, the phonon thermal conductivity. When simulating bulk material this can be looked up from literature values. When extending the model with nano inclusions this is no longer valid and it needs to be modeled too. A good and simple alternative or starting point for this could be [4], though better models exists.

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