

Homework Week 5: Recent Advances in Thermoelectric Materials and Physics Thermoelectricity: From Atoms to Systems

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Answer the **14 questions** including sub-questions below by choosing **one, best answer**. This homework does not count toward the final score, but solving and understanding this homework will be extremely helpful for passing the exam. Several homework problems are developed to help you familiarize with the third nanoHUB-U simulation tool (Thermoelectric material properties simulation tool based on the linearized Boltzmann transport equations).

1. **Differential conductivity and Seebeck coefficient – electrical conductivity trade-off** In a single nonparabolic band structure model, the electron dispersion relation is described as

$$E(1 + \alpha E) = \frac{\hbar^2 k^2}{2m^*} \quad (1)$$

where E is the electron energy, k is the electron wavevector, α is the non-parabolicity, and m^* is the effective mass at the band edge.

Electron transport and thermoelectric properties of a bulk semiconductor material can be calculated from the Boltzmann transport equation (BTE) under the relaxation time approximation. They are all integral functions of the *differential conductivity (Transport Distribution Function)*,

$$\sigma_d(E) = e^2 \tau(E) v^2(E) \rho_{DOS}(E) \left(-\frac{\partial f_0}{\partial E} \right) \quad (2)$$

Where e is the electron charge, $\tau(E)$ is the electron relaxation time or scattering time that is only a function of energy, $v(E)$ is the electron velocity in one direction, $\rho_{DOS}(E)$ is the density of states, and $f_0(E)$ is the Fermi-Dirac distribution. $(-\partial f_0 / \partial E)$ is the Fermi window. Note that the terms before the Fermi window in differential conductivity is identical to the $M(E)T(E)$ product, with a constant multiplication factor, in the Landauer formalism in diffusive transport limit, which you learned during the week 2 lectures in this course.

The electrical conductivity σ is simply an integral of the differential conductivity over energy, and the mobility μ is related to the electrical conductivity by $\sigma = ne\mu$, where n is the carrier concentration,

$$\sigma = \int_0^{\infty} \sigma_d(E) dE, \quad (3)$$

$$\mu = \frac{1}{e} \frac{\int_0^{\infty} \sigma_d(E) dE}{n}, \quad (4)$$

$$n = \int_0^{\infty} \rho_{DOS}(E) f_0(E) dE, \quad (5)$$

where E_F is the Fermi level relative to the band edge. The Seebeck coefficient S and the electronic thermal conductivity κ_e are given, respectively, by

$$S = -\frac{1}{eT} \frac{\int_0^{\infty} \sigma_d(E)(E - E_F) dE}{\int_0^{\infty} \sigma_d(E) dE}, \quad (6)$$

$$\kappa_e = \frac{1}{e^2 T} \int \sigma_d(E)(E - E_F)^2 dE - S^2 \sigma T. \quad (7)$$

All of these integrals can be directly written in the electron momentum space (k-space). Care should be taken when variables are changed from momentum to energy as often integration over transverse momentum is performed in one-dimensional transport. Now, we can calculate the thermoelectric properties by solving these Boltzmann transport equations for a given band structure. The thermoelectric material properties simulation tool at <https://nanohub.org/tools/btesolver> allows us to do these calculations, providing convenient graphical user interfaces for band structure inputs and various simulation options. Visit the link and run the simulation tool to answer the following questions.

1-1. Here we simulate n-type InGaAlAs alloys using the simulation tool. In the first phase of the simulation tool, select “n-InGaAlAs – n-type Indium Gallium Aluminum Arsenide” in the topmost material selection pull-down menu. The band structure configuration and the figure will be automatically updated. The valence bands are ignored here to calculate the electron transport only, and the second conduction band is much higher than the first conduction band, so it is also ignored here. Click the blue button beside the **Primary Conduction Band** label in the figure to check the band information of the first conduction band. Check that the effective mass and non-parabolicity are a function of the fractional composition x , which is the aluminum content in $(\text{In}_{0.53}\text{Ga}_{0.47}\text{As})_{1-x}(\text{In}_{0.52}\text{Al}_{0.48}\text{As})_x$ configuration (this particular quaternary composition is lattice matched to InP substrate). Enter “0” in the “**x (fraction of composition)**” box below the figure, so that you can simulate the ternary alloy $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ without Al.

Select “n-InGaAlAs – n-type Indium Gallium Aluminum Arsenide”

1 Band Structure 2 Scattering Properties 3 Simulation Parameters 4 Simulate

Material: n-InGaAlAs - n-type Indium Gallium Aluminum Arsenide

Bands: 1. Single Conduction Band - No Valence Bands

Here we simulate n-type $(\text{In}_{0.53}\text{Ga}_{0.47}\text{As})_{1-x}(\text{In}_{0.52}\text{Al}_{0.48}\text{As})_x$ alloy. This III-V semiconductor alloy has the primary conduction band at the Gamma valley in the Brillouin zone. Although this material also has a valence band at the Gamma valley, we ignore the valence band in this simulation to focus only on electron transport. Enter the Al content x in the Fractional Composition box below the band figure.

Primary Conduction Band

Enter “0” for x

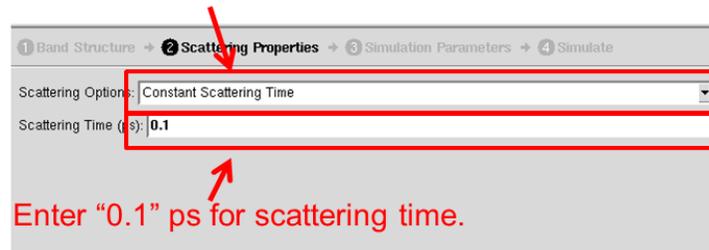
Fractional composition? yes

x (fraction of composition): 0

Scattering Properties >

In the next phase “**Scattering Properties**”, select “**Constant Scattering Time**” in the “**Scattering Options**” menu, and enter “**0.1**” (ps) for “**Scattering Time (ps)**”.

Select “Constant Scattering Time” option



In the next phase “**Simulation Parameters**”, select “**Differential Conductivity Analysis**” in the “**Analysis type**” menu. Below the menu, check that the type of carrier concentration is Electron as there is only a conduction band. Enter “**0**” eV for **Fermi level**, “**0**” eV for **Cut-off energy level** (we don’t use the cut-off in this simulation), and “**300**” K for **Temperature**. Enter “**4.0**” W/mK for the **lattice thermal conductivity** at this temperature. Then click “**Simulate**” to start simulation.

After the simulation is done, check the differential conductivity and density of states curves as a function of electron energy, and the resulting thermoelectric properties for this condition.

What are the Seebeck coefficient and the electrical conductivity of the $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ semiconductor at 300 K according to the simulation? Note that the actual values for real $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ can be different as we used a constant scattering time of 0.1 ps for simplicity in the first step.

- a. $S = -82.5 \mu\text{V/K}$, $\sigma = 1005.7 \Omega^{-1} \text{cm}^{-1}$
- b. $S = -142.5 \mu\text{V/K}$, $\sigma = 505.7 \Omega^{-1} \text{cm}^{-1}$
- c. $S = -182.5 \mu\text{V/K}$, $\sigma = 205.7 \Omega^{-1} \text{cm}^{-1}$
- d. $S = -242.5 \mu\text{V/K}$, $\sigma = 105.7 \Omega^{-1} \text{cm}^{-1}$
- e. $S = -312.5 \mu\text{V/K}$, $\sigma = 85.7 \Omega^{-1} \text{cm}^{-1}$

1-2. Repeat the simulation with a different **Fermi level** of **0.1 eV** this time while keeping all the other parameters unchanged from the previous simulation.

What are the Seebeck coefficient and the electrical conductivity now? Check how the two properties have changed with increasing Fermi level. Note that the electrical conductivity is the total area under the differential conductivity vs. energy curve, and the magnitude of the Seebeck coefficient is proportional to average energy of electrons contributing to differential conductivity with respect to the Fermi level.

- a. $S = -95.0 \mu\text{V/K}$, $\sigma = 843.2 \Omega^{-1} \text{cm}^{-1}$
- b. $S = -132.1 \mu\text{V/K}$, $\sigma = 515.3 \Omega^{-1} \text{cm}^{-1}$
- c. $S = -192.3 \mu\text{V/K}$, $\sigma = 201.4 \Omega^{-1} \text{cm}^{-1}$
- d. $S = -242.5 \mu\text{V/K}$, $\sigma = 105.7 \Omega^{-1} \text{cm}^{-1}$
- e. $S = -332.7 \mu\text{V/K}$, $\sigma = 85.1 \Omega^{-1} \text{cm}^{-1}$

1-3. Now, go back to the third phase “**Simulation parameters**” and switch the Analysis type to “**Varying carrier concentration at a constant temperature**”. Set “**1e17**” (cm^{-3}), “**1e19**” (cm^{-3}), and “**40**” for **Minimum carrier concentration**, **Maximum carrier concentration**, and **Number of carrier concentration data points**, respectively. Keep the temperature at **300 K** as well as all the other parameters. Then Run the simulation.

After the simulation is done, check how the electrical conductivity and the Seebeck coefficient vary with carrier concentration in the “**Electrical conductivity and Seebeck coefficient vs Concentration**” plot in the output phase. Note that increasing carrier concentration means increasing Fermi level. Due to the trade-off between the two properties, there is a maximum power factor at an optimal carrier concentration. What is the maximum power factor at this temperature and what is the optimal carrier concentration?

- a. $PF_{\max} = 6.02 \mu\text{W}/\text{cmK}^2$ at $n = 8.4 \times 10^{17} \text{ cm}^{-3}$
- b. $PF_{\max} = 8.02 \mu\text{W}/\text{cmK}^2$ at $n = 8.4 \times 10^{17} \text{ cm}^{-3}$
- c. $PF_{\max} = 10.02 \mu\text{W}/\text{cmK}^2$ at $n = 6.6 \times 10^{17} \text{ cm}^{-3}$
- d. $PF_{\max} = 12.02 \mu\text{W}/\text{cmK}^2$ at $n = 6.6 \times 10^{17} \text{ cm}^{-3}$
- e. $PF_{\max} = 14.02 \mu\text{W}/\text{cmK}^2$ at $n = 1.3 \times 10^{18} \text{ cm}^{-3}$

1-4. (continued from Prob. 1-3) Check that the ZT is also maximized at an optimal carrier concentration in the previous simulation. Regarding the ZT optimization, which of the following statements is correct?

- a. The optimal carrier concentration that maximizes ZT is the same as the optimal carrier concentration that maximizes the power factor because the lattice thermal conductivity is fixed with varying the carrier concentration.
- b. The optimal carrier concentration that maximizes ZT is higher than the optimal carrier concentration that maximizes the power factor because the electronic thermal conductivity decreases with increasing carrier concentration.
- c. The optimal carrier concentration that maximizes ZT is lower than the optimal carrier concentration that maximizes the power factor because the electronic thermal conductivity increases with increasing carrier concentration.
- d. The optimal carrier concentration that maximizes ZT is lower than the optimal carrier concentration that maximizes the power factor because the electronic thermal conductivity decreases with increasing carrier concentration.
- e. None of the above

2. **(Influence of a secondary conduction band)** While keeping the primary conduction band of the n-type InGaAs material in the simulation tool, add a secondary conduction band in the band structure to create an imaginary material with two conduction bands by selecting **“4. Double Conduction Bands – No Valence Bands”** in the **Bands** menu below the material selection menu in the first phase of the simulation tool. The band figure will be updated with a secondary conduction band added.

Click on the blue button beside **“Conduction band offset”** in the figure to enter **“0.1”** eV for the band offset between the two conduction bands. Then click on the other blue button beside **“Secondary Conduction Band”** to enter **“0.1”** (\times stationary electron mass m_0) for the **electron effective mass of the second band**, **“0”** for the **nonparabolicity**, and **“1”** for the **band degeneracy**.

Select **“4. Double Conduction Bands – No Valence Bands”** option

Here we simulate n-type $(\text{In}_{0.53}\text{Ga}_{0.47}\text{As})_{1-x}(\text{In}_{0.52}\text{Al}_{0.48}\text{As})_x$ alloy. This III-V semiconductor alloy has the primary conduction band at the Gamma valley in the Brillouin zone. Although this material also has a valence band at the Gamma valley, we ignore the valence band in this simulation to focus only on electron transport. Enter the Al content x in the Fractional Composition box below the band figure.

Change values...
 Electron effective mass of 2nd conduction band: 0.1
 Nonparabolicity for 2nd conduction band (1/eV): 0
 Band degeneracy of 2nd conduction band: 1

Primary Conduction Band
 Secondary Conduction Band
 Conduction Band Offset

Fractional composition?: no yes
 x (fraction of composition): 0

Scattering Properties >

Keep the **constant scattering time** at **“0.1”** ps, **Fermi level** at **“0.1”** eV, and **temperature** at **“300”** K in the second and third phases. Run the simulation for differential conductivity analysis.

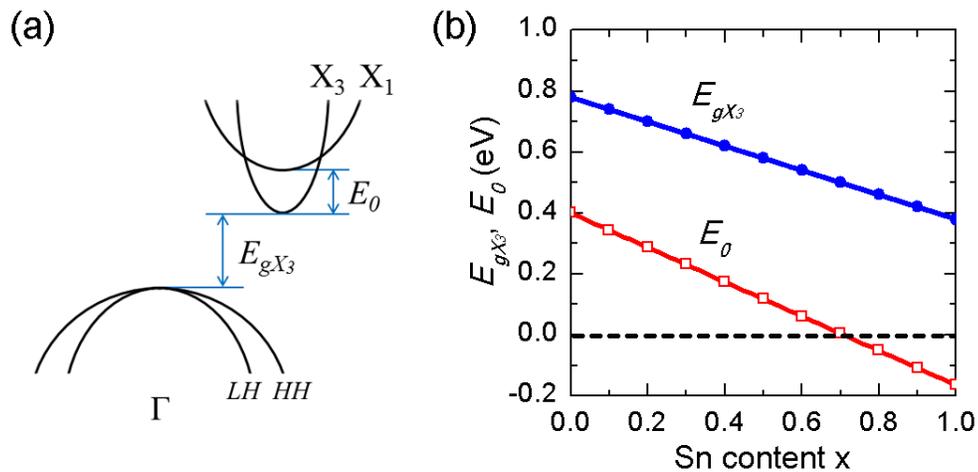
2-1. What are the Seebeck coefficient and the electrical conductivity for this material according to the simulation?

- a. $S = -67.3 \mu\text{V/K}$, $\sigma = 1013.8 \Omega^{-1} \text{cm}^{-1}$
- b. $S = -95.0 \mu\text{V/K}$, $\sigma = 843.2 \Omega^{-1} \text{cm}^{-1}$
- c. $S = -95.0 \mu\text{V/K}$, $\sigma = 645.7 \Omega^{-1} \text{cm}^{-1}$
- d. $S = -120.1 \mu\text{V/K}$, $\sigma = 843.2 \Omega^{-1} \text{cm}^{-1}$
- e. $S = -120.1 \mu\text{V/K}$, $\sigma = 1013.8 \Omega^{-1} \text{cm}^{-1}$

2-2. Compare these values of the Seebeck coefficient and the electrical conductivity with those obtained in Prob. 1-2 in the case where there was no secondary band. Which of the following statements is correct?

- a. The Seebeck coefficient decreased due to the existence of the secondary conduction band because of additional scattering.
- b. The Seebeck coefficient increased because the secondary band increased the differential conductivity above the Fermi level while the differential conductivity below the Fermi level remained the same, so that the degree of asymmetry of the differential conductivity around the Fermi level increased.
- c. The electrical conductivity decreased because the Seebeck coefficient increased by the influence of the secondary band and there is a trade-off between the Seebeck coefficient and the electrical conductivity.
- d. The electrical conductivity increased because the secondary band added more states within the Fermi window.
- e. a and c
- f. a and d
- g. b and c
- h. b and d

3. (Band convergence in $\text{Mg}_2\text{Sn}_x\text{Si}_{1-x}$ solid solutions) $\text{Mg}_2\text{Sn}_x\text{Si}_{1-x}$ solid solutions have recently attracted a lot of attention as a cheap, environmental-friendly, and efficient thermoelectric material in the mid-temperature range of 500 ~ 900 K. This alloy material has two conduction valleys in the X-point in the Brillouin zone, and multiple valence valleys overlapped at the Γ -point as shown in the Figure (a) below. The band gap between the primary conduction band and the valence bands, and the band offset between the two conduction bands are a function of Sn content x . It is assumed that the x dependences of the band gap and conduction band offset are linear as shown in the figure (b) below.



The band structure information for $\text{Mg}_2\text{Sn}_x\text{Si}_{1-x}$ is included as a function of Sn content x as well as temperature in the material library in the thermoelectric material properties simulation tool (<https://nanohub.org/tools/btesolver>). To simulate the $\text{Mg}_2\text{Sn}_x\text{Si}_{1-x}$ solid solutions, select “**Mg2SnSi – Magnesium Tin Silicide**” in the material selection menu in the first phase of the simulation tool. The band structure figure and parameters will be automatically updated. Two conduction bands and two valence bands are fully included in the band structure with appropriate parameters that are chosen to fit best the experimental data from the literature.

In the second phase “**Scattering properties**”, make sure to select “**Energy-Dependent Scattering Time**” option in the **Scattering Option**. Real material parameters such as lattice constant and dielectric constants are already inserted in the input boxes. The major scattering mechanisms in this material are “**Enabled**” in each of the scattering boxes to include the realistic energy-dependent scattering time in the Boltzmann transport calculations. The **acoustic phonon deformation potential scattering** is a predominant scattering mechanism in this material. The **ionized impurity scattering** and the **polar optical phonon scattering** are also included for the transport calculations. Note that some of the

material and scattering parameters are a function of Sn content x . Keep all the values in the input boxes for the simulations.

Calculate the thermoelectric properties of the **n-type** $\text{Mg}_2\text{Sn}_x\text{Si}_{1-x}$ at **700 K** with varying **electron concentration** from **$1\text{e}19$** to **$1\text{e}21$** cm^{-3} . Repeat the calculations for various Sn contents **$x = 0.2, 0.4, 0.6, 0.8,$** and **1.0** . Use a constant lattice thermal conductivity of **1.2** **W/mK** for all the compositions.

3-1. Which Sn content can achieve the largest ZT at 700 K, and what is the corresponding maximum ZT of this alloy at 700 K? Choose the closest values.

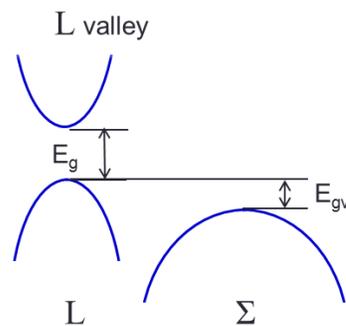
- a. $x = 0.2, ZT_{\text{max}} = 0.9$
- b. $x = 0.4, ZT_{\text{max}} = 1.0$
- c. $x = 0.6, ZT_{\text{max}} = 1.1$
- d. $x = 0.8, ZT_{\text{max}} = 1.2$
- e. $x = 1.0, ZT_{\text{max}} = 0.9$
- f. All the compositions have the same $ZT_{\text{max}} = 1.2$.

3-2. Check all the plots, e.g. Seebeck coefficient, electrical conductivity, and thermal conductivity plots, carefully for various Sn contents, and identify all of the major reasons ZT is maximized at a particular Sn content chosen in the previous question.

- a. Large Seebeck coefficients due to the larger separation of the two conduction bands
- b. Large Seebeck coefficients due to the convergence of the two conduction bands
- c. Large electrical conductivity due to the relatively lighter effective mass
- d. Large electrical conductivity due to the relatively heavier effective mass
- e. Smaller electronic thermal conductivity due to the smaller lattice thermal conductivity
- f. Smaller electronic thermal conductivity due to the smaller bipolar electronic thermal conductivity with a larger band gap
- g. a and c
- h. a and e
- i. a and f
- j. b and c
- k. b and e
- l. b and f

4. **(Doping optimization of p-type PbTe)** PbTe has been known since 1960s as an excellent thermoelectric material in the mid-temperature range. Recently, a great deal of research efforts has been done world-wide on nanostructured PbTe-based materials to further improve the thermoelectric performance of PbTe. In order to enhance the figure of merit, however, doping optimization of the material is needed. It is helpful to understand the impact of doping on TE properties of base PbTe material.

PbTe has a direct band gap at temperatures below 450 K with both the conduction band and the valence band at the L valley in the Brillouin zone. The second valence band is located at the Σ valley. The band gap increases linearly with temperature while the band offset between the two valence band edges slowly decreases with temperature. Above 450 K or so, the L and Σ valley valence bands converge, and the Σ valley becomes the primary valence band as its band edge becomes higher than that of the L valley. All the effective masses and the nonparabolicities of the bands are temperature-dependent. These band parameters are given in the simulation tool.



Band structure of PbTe

In this problem, we use the thermoelectric material properties simulation tool to optimize the p-type doping concentration of PbTe at two different temperatures: 600 K and 900 K. Use the energy-dependent scattering time for the realistic estimation of the thermoelectric properties. Acoustic and optical phonon deformation potential scatterings are dominant scattering mechanisms in PbTe. Polar optical phonon scattering is also strong as the ratio between the static and high-frequency dielectric constants of PbTe is very large.

4-1. Assume a constant lattice thermal conductivity of **1.2 W/mK** for doping optimization of PbTe at **600 K**. Find the optimal hole concentration (h_{opt}) that maximizes the ZT value at 600 K, and the corresponding maximum ZT value using the simulation tool.

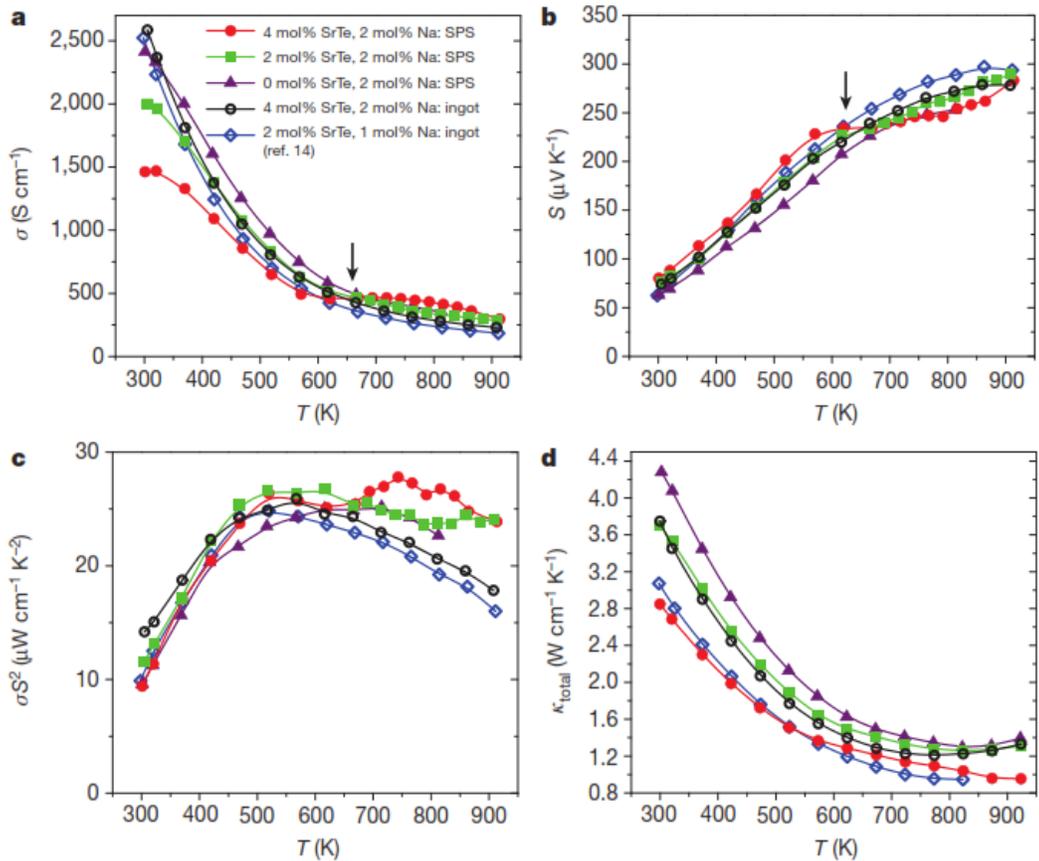
- a. $ZT_{max} = 1.21$ at $h_{opt} = 9.1e18 \text{ cm}^{-3}$
- b. $ZT_{max} = 1.41$ at $h_{opt} = 4.5e19 \text{ cm}^{-3}$
- c. $ZT_{max} = 1.61$ at $h_{opt} = 7.6e19 \text{ cm}^{-3}$
- d. $ZT_{max} = 1.71$ at $h_{opt} = 9.6e19 \text{ cm}^{-3}$
- e. $ZT_{max} = 1.91$ at $h_{opt} = 1.4e20 \text{ cm}^{-3}$

4-2. Use a constant lattice thermal conductivity of **1.0 W/mK** for doping optimization of PbTe at **900 K**. Note that the lattice thermal conductivity typically decreases with increasing temperature in this temperature range due to the increased Umklapp scattering. Find the optimal hole concentration (h_{opt}) that maximizes the ZT value at 900 K, and the corresponding maximum ZT value using the simulation tool.

- a. $ZT_{max} = 1.25$ at $h_{opt} = 1.4e20 \text{ cm}^{-3}$
- b. $ZT_{max} = 1.49$ at $h_{opt} = 2.2e20 \text{ cm}^{-3}$
- c. $ZT_{max} = 1.74$ at $h_{opt} = 3.5e20 \text{ cm}^{-3}$
- d. $ZT_{max} = 1.91$ at $h_{opt} = 1.3e20 \text{ cm}^{-3}$
- e. $ZT_{max} = 2.20$ at $h_{opt} = 1.5e20 \text{ cm}^{-3}$

5. (Analysis of the SPS-ed Na-doped PbTe:SrTe with $ZT \sim 2.2$) Recently it has been reported that a spark-plasma-sintered Na-doped PbTe:SrTe (4% Sr) was measured to have a $ZT \sim 2.2$ at 915 K. (See Biswas et al., *Nature* **489**, 414, 2012.) In this homework problem, we attempt to analyze the experimental data from the paper using the simulation tool. Note that as the material contains 4 % Sr as well as 2 % Na, our simulations based on pure PbTe is a first order approximation. Since you will see that the match between theory and experiment is reasonably good, one can conclude that the “electronic” properties of the nanostructured material are quite close to pure PbTe while additional phonon scattering has improved ZT significantly.

The figure below shows the experimental data from the paper. In the paper, only a room temperature hole concentrations of the samples were experimentally measured. The best sample with $ZT \sim 2.2$ (the red curve in the figure below) was measured to have a $9 \times 10^{19} \text{ cm}^{-3}$ hole concentration at room temperature. However, the hole concentration is expected to increase as temperature increases in this sample as the author anticipated by the fact that the Na atoms diffuses more into the matrix from the grain boundaries where the Na atoms are mostly electrically inactive to donate more holes to the matrix at higher temperatures.



5-1. Assuming that the Seebeck coefficient does not change significantly by nanostructuring in the material, find an estimated range of the hole concentration at 900 K for the best sample of the paper. (Hint: Find the range of hole concentration where the Seebeck coefficient is close to the experimental value of the sample at 900 K using the previous PbTe doping optimization simulations conducted in Prob. 4-2.)

- a. between $2.0 \times 10^{19} \text{ cm}^{-3}$ and $3.0 \times 10^{19} \text{ cm}^{-3}$
- b. between $9.0 \times 10^{19} \text{ cm}^{-3}$ and $1.5 \times 10^{20} \text{ cm}^{-3}$
- c. between $1.5 \times 10^{20} \text{ cm}^{-3}$ and $3.0 \times 10^{20} \text{ cm}^{-3}$
- d. between $3.0 \times 10^{19} \text{ cm}^{-3}$ and $4.5 \times 10^{20} \text{ cm}^{-3}$
- e. between $4.5 \times 10^{19} \text{ cm}^{-3}$ and $6.0 \times 10^{20} \text{ cm}^{-3}$

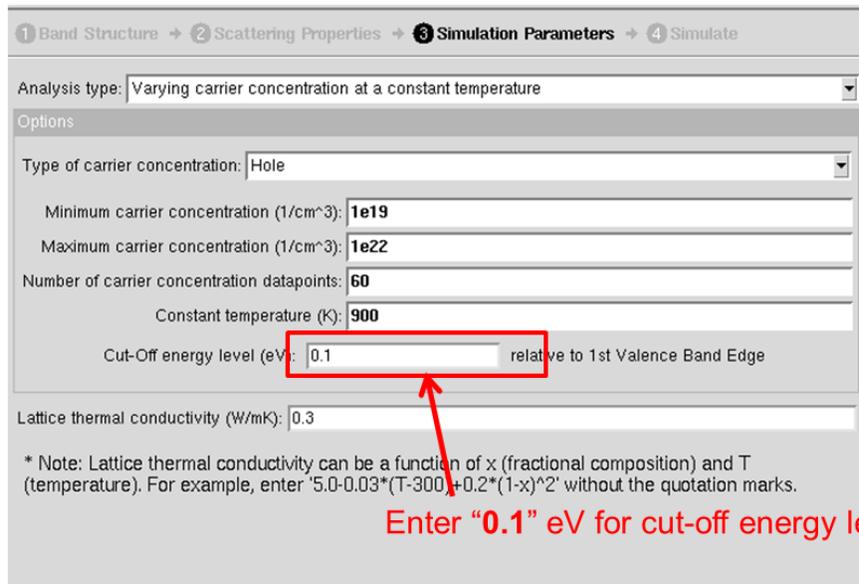
5-2. What is the range of the electrical conductivity of PbTe at 900 K for the hole concentration range obtained in Prob. 5-1 based on the simulation? Why is there a discrepancy with the experimental data from the paper?

- a. Between 150 and $200 \text{ } \Omega^{-1} \text{ cm}^{-1}$. The experimental data is slightly higher because the SrTe content reduces the mobility.
- b. Between 200 and $280 \text{ } \Omega^{-1} \text{ cm}^{-1}$. The experimental data is slightly higher because the Na impurity scattering is weaker than the conventional impurity scattering.
- c. Between 280 and $400 \text{ } \Omega^{-1} \text{ cm}^{-1}$. The experimental data is slightly lower because the nanostructures and grain boundaries reduce the electrical conductivity by additional carrier scattering.
- d. Between 400 and $550 \text{ } \Omega^{-1} \text{ cm}^{-1}$. The experimental data is lower because the nanostructures and grain boundaries reduce the electrical conductivity with additional carrier scattering.
- e. Between 550 and $700 \text{ } \Omega^{-1} \text{ cm}^{-1}$. The experimental data is much lower because the nanostructures significantly reduce the electrical conductivity with additional carrier scattering.

5-3. What is the estimated electronic thermal conductivity for the sample? How much does the bipolar thermal conductivity contribute to the total electronic thermal conductivity? Finally, find the lattice thermal conductivity at 900 K using the experimental total thermal conductivity value from the paper.

- a. $\kappa_e = 0.5 \text{ W/mK}$, $\kappa_{bi} = 0.2 \text{ W/mK}$, and $\kappa_l = 0.5 \text{ W/mK}$
- b. $\kappa_e = 0.6 \text{ W/mK}$, $\kappa_{bi} = 0.3 \text{ W/mK}$, and $\kappa_l = 0.4 \text{ W/mK}$
- c. $\kappa_e = 0.7 \text{ W/mK}$, $\kappa_{bi} = 0.3 \text{ W/mK}$, and $\kappa_l = 0.3 \text{ W/mK}$
- d. $\kappa_e = 0.8 \text{ W/mK}$, $\kappa_{bi} = 0.4 \text{ W/mK}$, and $\kappa_l = 0.2 \text{ W/mK}$
- e. $\kappa_e = 0.9 \text{ W/mK}$, $\kappa_{bi} = 0.5 \text{ W/mK}$, and $\kappa_l = 0.1 \text{ W/mK}$

6. (Carrier energy filtering in PbTe) When there is a cut-off energy level in the carrier transport, below which all the carriers are prevented from participating in the transport, a significant enhancement of the thermoelectric figure of merit in a bulk material is possible. This is often called, energy filtering. The enhancement comes from two effects: a large enhancement of Seebeck coefficient due to the enhanced asymmetry in the differential conductivity as shown in Prob. 1, and a large reduction of electronic thermal conductivity due to the reduced electrical conductivity by the electron energy filtering. The electrical conductivity is indeed reduced by the filtering effect because the total number of carriers participating in the conduction is reduced by the cut-off process. However, the enhancement of the Seebeck coefficient can be much larger than the electrical conductivity reduction if the cut-off energy level is appropriately selected for the carrier concentration in the material or an appropriate carrier concentration is selected for a fixed cut-off energy level. See [Bahk et al., *Phys. Rev. B* **87**, 075204 (2013)] for more information.



Set the **cut-off energy level** to be “**0.1**” eV above the primary valence band edge in p-type PbTe at 900 K. Find the optimal doping concentration that maximizes ZT for the PbTe under the filtering effect at 900 K, and the corresponding maximum ZT by the filtering effect with a 0.1 eV cut-off? Use the lattice thermal conductivity value obtained from Prob. 5-3.

a. $ZT_{\max} = 1.5$ at $n_{\text{opt}} = 1.6 \times 10^{20} \text{ cm}^{-3}$

b. $ZT_{\max} = 2.0$ at $n_{\text{opt}} = 2.1 \times 10^{20} \text{ cm}^{-3}$

c. $ZT_{\max} = 2.7$ at $n_{\text{opt}} = 3.4 \times 10^{20} \text{ cm}^{-3}$

d. $ZT_{\max} = 3.8$ at $n_{\text{opt}} = 5.3 \times 10^{20} \text{ cm}^{-3}$

e. $ZT_{\max} = 4.9$ at $n_{\text{opt}} = 7.6 \times 10^{20} \text{ cm}^{-3}$