Exercise: Week 2 Bonus Lecture
Thermoelectric Materials and Devices
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This exercise is not graded, and is intended for those who wish to learn more about thermoelectric (TE) calculations using full band dispersions of electrons and phonons.

This exercise asks you to reproduce many of the results and figures presented in the Bonus Lecture. This will require running the TE simulator **LanTraP** (a full band TE simulator for electrons/phonons that handles ballistic, quasi-ballistic and diffusive transport regimes) which is available online at:

nanohub.org/resources/lantrap

on the nanoHUB website. Note that the tool is hosted and launched online, and does not need to be downloaded.

To begin, from the main webpage of the tool, click on the "**Supporting Docs**" tab. Here, users can download two zipped files entitled: "**electron_dispersions.zip**" and "**phonon_dispersions.zip**". Once unzipped, the user will find several text files containing the full band *electron* and *phonon* dispersions (e.g. parabolic band, electron Si, electron Bi_2Te_3, Debye model, phonon Si, …).

Note that on the "**Supporting Docs**" webpage, there is "**TutorialCases.pdf**" that walks through each example and explains in a step-by-step manner how to run LanTraP. There is also "**UserManual.pdf**" which describes the function and meaning of each input parameter, as well as the specific format of the input dispersion files.

1) In the Bonus Lecture, on slide 10 it was explained that the electronic distribution of modes depends on the dimensionality of the system (e.g. 1D: nanowire, 2D: film, 3D: bulk). Follow the steps in section **A.1**, **A.5** and **A.6** in the Tutorial document to calculate the distribution of modes in the case of 1D, 2D and 3D parabolic bands ($E = \hbar k^2 / 2m^*$, where E is the electron energy, k is the norm of the reciprocal lattice vector, m^* is the effective mass and $h = 2\pi\hbar$ is Planck's constant). The dispersion data files are located in the zipped file and do not need to be prepared. Confirm that you obtain the same trend as the plots presented on slide 10, and that your calculations match the analytical expressions on slide 10.

2) Calculate the distribution of modes for a realistic electronic dispersion, that of Bi_2Te_3. The electronic dispersion of Bi_2Te_3 included in the zipped is the same that presented on slide 11 in the Bonus Lecture. Follow the step in section **A.8** of the Tutorial to extract the distribution of modes of Bi_2Te_3, and compare your result to the $M_{3D}(E)$

(continued on next page)

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shown on slide 11.

3) Using the Bi_2Te_3 $M_{3D}(E)$ calculated in the previous step (which can be downloaded, and used as an input), and assuming the valence band mean-free-path for backscattering (MFP) is 15 nm and the conduction band MFP is 21 nm, compute the bulk TE coefficients. Compare your results to the electronic conductivity σ, Seebeck coefficient S and electronic thermal conductivity κ_e presented on slides 16, 17 and 18 in the Bonus Lecture.

4) Calculate the phonon distribution of modes for a simple Debye model ($E = \hbar \upsilon_s |k|$, where E is the phonon energy, υ_s is the speed of sound and $|k|$ is the norm of the reciprocal lattice vector). Note that the dispersion data file is located in the zipped file, and does not need to be prepared. Follow the steps in section **B.1** in the tutorial. Verify that the extracted distribution of modes is equal to $M_{\text{Debye}}(E) = 3E^2 / 4\pi\hbar^2\upsilon_s^2$ (note that the factor of three appears from the fact that there are always three acoustic phonon braches).

5) Next, calculate the phonon distribution of modes and lattice thermal conductivity of Si. Follow the steps in section **B.2** of the tutorial. You should find a lattice thermal conductivity of ≈ 140 W/m-K at room temperature, which corresponds to the experimental value. (Note that the lattice thermal conductivity of Bi_2Te_3 is ≈ 1.4 W/m-K at room temperature. This difference in κ_L is the reason why Bi_2Te_3 is a far better room temperature TE than Si.)

   In this case, you can simply input a constant MFP of 141 nm, which represents the average MFP previously calibrated to match the experimental lattice thermal conductivity of Si. As mentioned in the Bonus Lecture, phonon MFPs often have a strong dependence on energy. **Hint:** if you wish to include your own specific energy-dependent MFP, simply (i) download the $M_{3D}(E)$, (ii) open, e.g. with Matlab, and multiply the distribution of modes by your specific MFP, (iii) save the data to a text file and (iiii) upload the distribution of modes - MFP product to the tool and perform a ballistic phonon TE calculation (ballistic since the MFP is already included in the data file). The same procedure applies for electrons, if a user wishes to include an energy-dependent MFP that is more complicated than a power law (which is already available in the tool).

End of exercise. This exercise contains 5 questions.