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PHONON DISPERSION AND RELAXATION TIME IN URANIUM DIOXIDE

by

Dallin C Parkinson

A report submitted in partial fulfillment
of the requirements for the degree

of

MASTER OF SCIENCE

in

Mechanical Engineering

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2017

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ABSTRACT

Phonon Dispersion and Relaxation Time in Uranium Dioxide

by

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Utah State University, 2017

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Department: Mechanical Engineering

Phonon dispersion branches are used to obtain an effective relaxation time to calculate thermal conductivity of Uranium Dioxide (UO_2). The method presented closely follows that of Deskins' [1] phonon-phonon interaction that uses a three-phonon process which satisfies momentum and energy conservation. All phonon branches including longitudinal acoustic, transverse acoustic, longitudinal optical and transverse optical are considered in the calculation of the relaxation time.

After one phonon is identified, a scan is initiated to test all phonon combinations that will satisfy the conservation equations. When the scan identifies a valid three-phonon combination a relaxation time is calculated for that combination. All the relaxation times from the possible combinations are summed using Mathias' rule to obtain a total approximate relaxation time for that phonon.

Thermal conductivity at equilibrium can be calculated at a specific temperature using the relaxation time approximation of the Boltzmann equation [2]. This approximation uses specific heat, relaxation time, group velocity and the Bose-Einstein

distribution.

Eventually, the goal of this work is to apply the routine for calculating relaxation time from this work to a Monte Carlo simulation that will treat systems not in equilibrium.

(23 Pages)

PUBLIC ABSTRACT

Phonon Dispersion and Relaxation Time in Uranium Dioxide

Dallin C. Parkinson

Utah State University, 2017

Phonons are lattice vibrations that are directly related to the thermal conductivity of materials. Work was done to model the thermal conductivity of Uranium Dioxide (UO_2) at equilibrium using a relaxation time approximation of the Boltzmann equation.

Phonon behavior depends on the polarization and the phase of each phonon. The main branches of phonons are longitudinal acoustic, transverse acoustic, longitudinal optical and transverse optical. For example, optical phonons have a higher frequency and consequently a higher energy and longitudinal phonons have a higher group velocity. Phonons are initialized and tested with a scanning routine to find all possible three-phonon combinations that will satisfy both momentum and energy conservation. These three-phonon combinations will be considered in calculating the relaxation time.

From the relaxation time approximation of the Boltzmann equation thermal conductivity can be determined as a function of temperature, specific heat, relaxation time and the Bose-Einstein distribution function.

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Dallin C. Parkinson

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INTRODUCTION

Because of the large potential of UO_2 to produce power, many experiments and studies have been conducted to better understand its properties to predict and improve performance in power production [3] [4]. Due to the radioactive and potentially hazardous nature of UO_2 there are limited locations and personnel that are capable and permitted to conduct experiments and further studies. Because of the limitations to physical experiments, many studies have been done to produce and improve models that can predict thermal properties. The Boltzmann equation is one of the main methods for modeling phonon transport [5].

$$\frac{\partial f}{\partial t} + V_g \cdot \Delta f = \left[\frac{\partial f}{\partial t} \right]_{scat} = \sum_{K'} [\Phi(K, K')f(K') - \Phi(K', K)f(K)]$$

1.1 Phonons

A lot of previous work has gone to show how phonons, or lattice vibrations, are related to thermal conductivity [2] [6] [7]. To visualize phonons, one can imagine atoms with their respective bonds within a lattice as a continuous system of masses and springs [8]. As one atom vibrates it will interact with the rest of the atoms within the lattice. This way phonons are treated essentially as particles although they can also exhibit wavelike behavior.

Phonons are the main contributors of thermal conductivity in non-conductive materials such as diamond. This example also proves that the phonon contribution to thermal conductivity is not negligible compared to the free electron contribution [8]. Having the ability to model phonon transport allows one to predict thermal conductivity [2]. There are two types of phonons, optical phonons and acoustic phonons. Phonons are

also classified by their polarization, the direction in which they vibrate, as either longitudinal or transverse. Phonons can scatter or interact with others through two main modes, Normal (N-process) scattering and Umklapp (U-process) scattering. Normal phonon scattering allows heat to flow through the lattice unrestricted [9]. If N-process were the only process of phonon interaction thermal conductivity would be infinite [1] [10]. Thermal conductivity is negatively related to Umklapp phonon scattering and decreases as U-process scattering increases [11].

1.2 BTE and the Monte Carlo Method

As mentioned above the Boltzmann Transport Equation is used to describe phonon behavior. The Boltzmann Equation is especially useful because it can model phonons at an equilibrium or non-equilibrium state [5]. However, this equation is difficult to solve and very expensive computationally. This leads to the interest in the Monte Carlo method which has been used for decades to give solutions to the Boltzmann Equation [5] [10] [12]. Using the Monte Carlo method, many instances of phonons are simulated with scattering occurring randomly based on probabilities often based on relaxation time [1] [5]. If enough phonons are simulated then the Monte Carlo Method results approach real world behavior [5]. Although this work does not treat the Monte Carlo method, the phonon dispersion and relaxation time calculations can be used in the development of a Monte Carlo code or the modification of the existing one developed by Dr. Roberts.

1.3 Relaxation time approximation

Work done by Holland resulted in an equation for thermal conductivity at equilibrium based on the Boltzmann equation.

$$\kappa = \frac{4\pi}{3} \frac{1}{(2\pi)^3} \sum_p \int [v_{Kp}^2 \tau(K,p) C_{ph}(K,p) f(K,p)] dK$$

This equation uses the relaxation time approximation to determine the scattering events [2]. More will be said about this equation later, but it is one way the relaxation time can be utilized without needing to use Monte Carlo simulation.

PHONON DISPERSION BRANCHES

To begin the treatment of phonon relaxation we need to know the phonon dispersion curves. Table 1 contains fitting parameters for each of the phonon polarizations to be used in a cubic equation. These fits were obtained from the work done by Dolling [13] and used in the study by Deskins [1]. Since phonons are lattice vibrations it is possible to obtain phonon dispersion data through several different methods including: neutron scattering [13] [14] [15], Raman spectroscopy [16] [17], and x-ray spectroscopy [18].

Table 1: Phonon dispersion branches. For the LA and LO branches the second row of fitting parameters corresponds to $K_{red} > 0.5$

<i>Branch</i>	$\frac{A}{2\pi}$	$\frac{B}{2\pi}$	$\frac{C}{2\pi}$	$\frac{D}{2\pi}$
<i>LA</i>	-5.00578×10^{-19}	-3.79652×10^{-8}	1035.08298	0
	1.77606×10^{-18}	-9.37422×10^{-8}	1450.4614	-9.77108×10^{11}
<i>TA</i>	-1.82517×10^{-18}	1.75603×10^{-8}	318.904326	0
<i>LO</i>	1.10738×10^{-18}	-1.08783×10^{-7}	0	1.34487×10^{13}
	1.64367×10^{-17}	-3.25511×10^{-7}	972.588976	1.20762×10^{13}
<i>TO</i>	2.11922×10^{-18}	-3.65102×10^{-8}	0	8.49391×10^{12}

These fits are used to calculate the frequency of each branch as a function of wavevector where $\omega(K) = AK^3 + BK^2 + CK + D$ [1]. It may be noted that the longitudinal branches have two sets of fitting parameters. The first set of fitting parameters is for when the reduced wavevector is less than half of the maximum wavevector (i.e. $K_{red} < 0.5$) the second set is for reduced wavevector values above

$K_{red} = 0.5$ where $K_{red} = K/K_{max}$. A branch switch function was created to set the right fitting parameters to each branch. The switch function is called for each phonon and assigns the fit values based on an input branch number and reduced wavevector and in turn sets the frequency. Figure 1 shows the dispersion curves for each of the branches as frequency as a function of the wavevector.

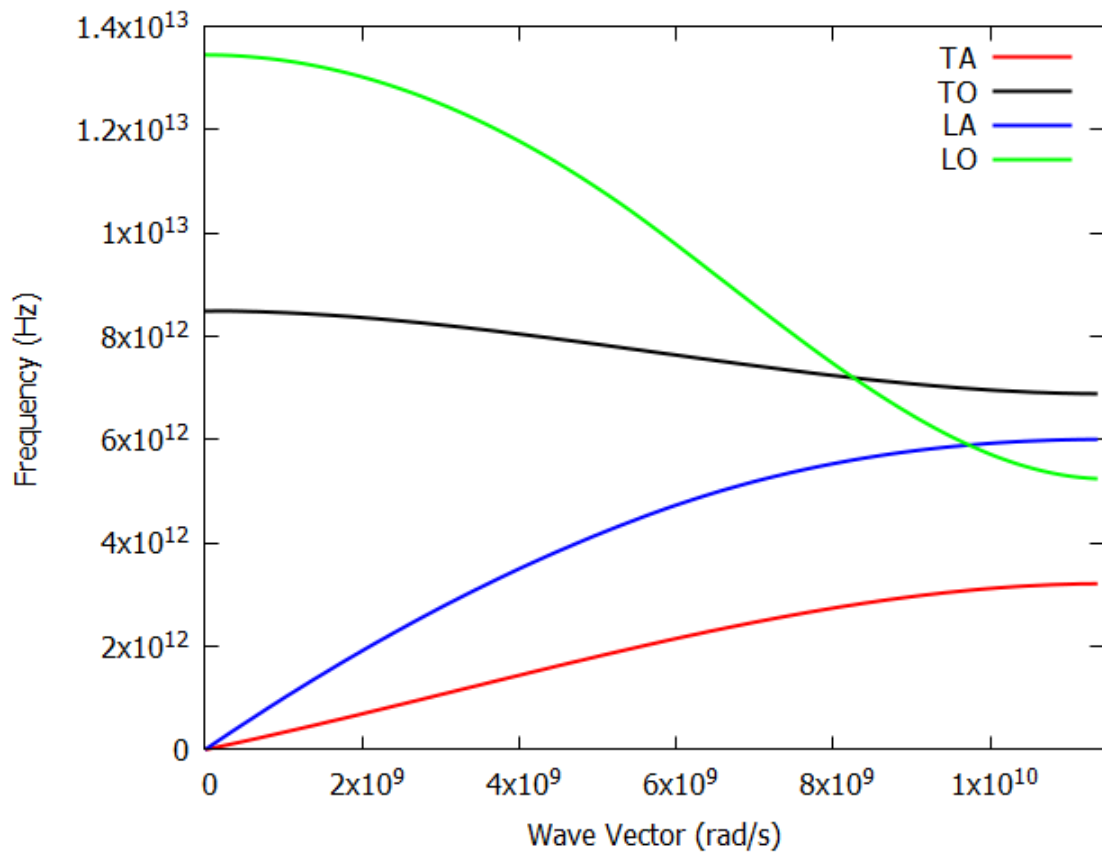


Figure 1: Dispersion Branches as obtained from the cubic fit of work done by Dolling.

CONSERVATION EQUATIONS AND PHONON BEHAVIOR

Phonon energy is defined as $\hbar\omega$ and, although phonons do not have actual physical momentum, $\hbar K$ is considered an equivalent phonon momentum [1] [9]. Two equations govern the possible scattering of phonons which will end up determining the relaxation times for the three-phonon process [1] [11].

Momentum conservation:

$$K + K' \leftrightarrow K'' + b \quad (3.1)$$

and Energy conservation:

$$\omega + \omega' \leftrightarrow \omega'' \quad (3.2)$$

where the term, b , is the reciprocal lattice vector.

When the scattering is within the first Brillouin zone the reciprocal lattice vector is set to zero and is considered an N-process scattering event. The first Brillouin zone has been defined in this work as any value of the wavevector between 0 and K_{max} . $K_{max} = \frac{2\pi}{a_o}$ with $a_o = 5.473\text{\AA}$. When the scan process results in a wavevector that exceeds the first Brillouin zone it becomes a U-process event. Phonon combinations falling outside the Brillouin zone can be seen in Figure 3 and Figure 5 as the curves arrive at K_{max} then reflect.

The conservation equations have a two-sided arrow that shows two phonons can combine to form one or that one phonon can decay into two separate phonons. The equations are not one directional.

SCAN ROUTINE

This chapter details the scan routine that identifies all possible phonon combinations that follow the conservation equations detailed in the previous chapter. It follows closely the scan outlines by Deskins [1].

A phonon is defined with a wavevector and branch number and its resulting frequency is calculated from the dispersion curves detailed in Chapter 1. The routine then initializes a secondary phonon loop and scans through all branches and wavevector values, adding them to the original phonon to obtain a third wavevector following the conservation equation $K + K' = K''$. During the scan of the secondary phonon the wavevector is used to calculate frequency with the cubic function $\omega'(K')$. After the primary and secondary phonons have an assigned branch, wavevector and frequency and the third phonon has an assigned branch and wavevector the frequency for the third phonon is calculated, $\omega''(K'')$.

If the third phonon falls outside the first Brillouin Zone the reciprocal lattice vector (b) no longer equals zero, and the scattering combination is counted as a U-process scattering event. Phonon combinations fall outside the Brillouin Zone when $K + K' > K_{max}$. The routine initializes b to zero and checks during the scan that the third phonon wave vector, K'' , is below K_{max} . When $K'' > K_{max}$ the reciprocal lattice vector is defined as:

$$b = K + K' - K_{max}$$

And the wave vector of the third phonon becomes:

$$K'' = K + K' - b$$

Conservation of energy is tested with equation 3.2. When the wavevectors and frequencies of the three phonons satisfy both conservations equations the resulting three-phonon combination is possible and is counted in the relaxation time calculation. To test that conservation of energy is satisfied a temporary variable $\Delta\omega$ is defined as:

$$\Delta\omega = \omega + \omega' - \omega''$$

The scan routine keeps track of $\Delta\omega$ and tests for a change in sign. When the sign changes that means $\Delta\omega = 0$ and the equation 3.2 is satisfied.

Summarized, the steps are:

1. Assign the primary phonon a frequency and wavevector.
2. Scan through secondary phonon wavevector.
 - a. Assign frequency of secondary phonon, $\omega'(K')$.
3. Add primary and secondary phonon wavevector to get third wavevector.

$$K + K' = K''$$

4. Assign frequency to third phonon, $\omega''(K'')$.
5. Calculate $\Delta\omega$ and test for change in sign.
6. When $\Delta\omega = 0$ keep the corresponding frequency of the third phonon ω'' .

The following figures show the results of the scan routine for the LA dispersion branch at $K_{red} = 0$ and $K_{red} = \frac{1}{3}$ as well as the TO dispersion branch at $K_{red} = 0$ and

$$K_{red} = \frac{1}{4}$$

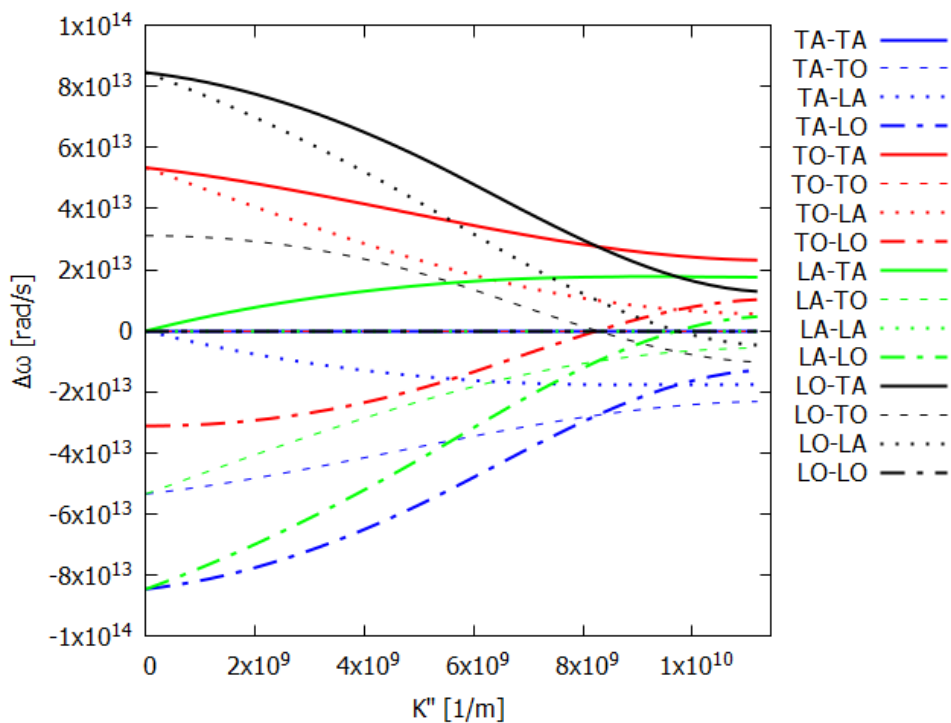


Figure 2: Scan results showing $\Delta\omega$ vs. K'' of an LA phonon at $K_{red} = 0$

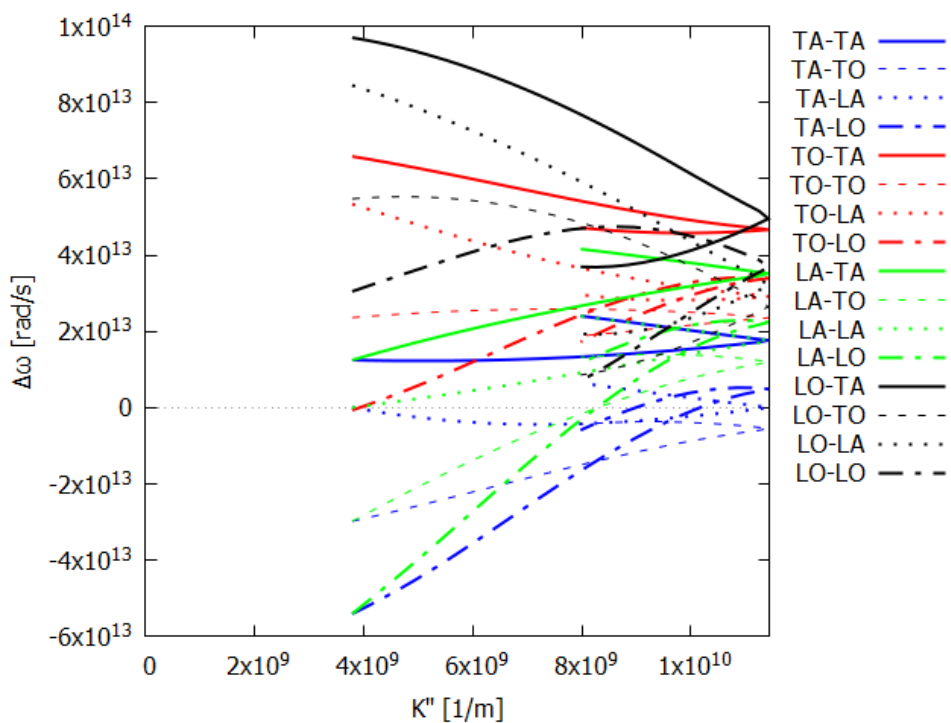


Figure 3: Scan results showing $\Delta\omega$ vs. K'' of an LA phonon at $K_{red} = \frac{1}{3}$

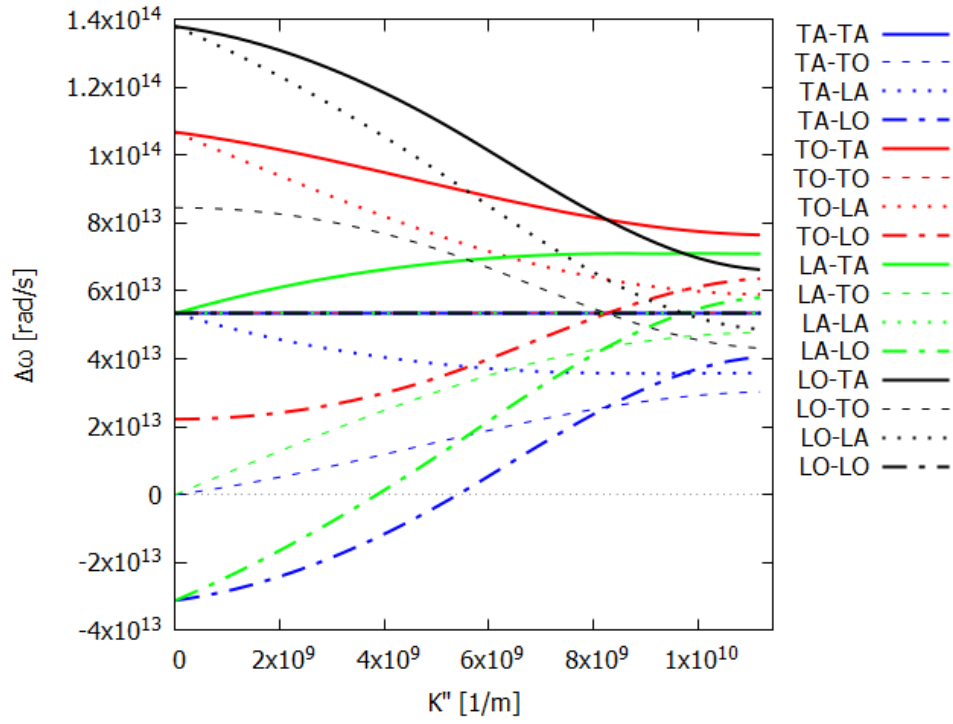


Figure 4: Scan results showing $\Delta\omega$ vs. K'' of a TO phonon at $K_{red} = 0$

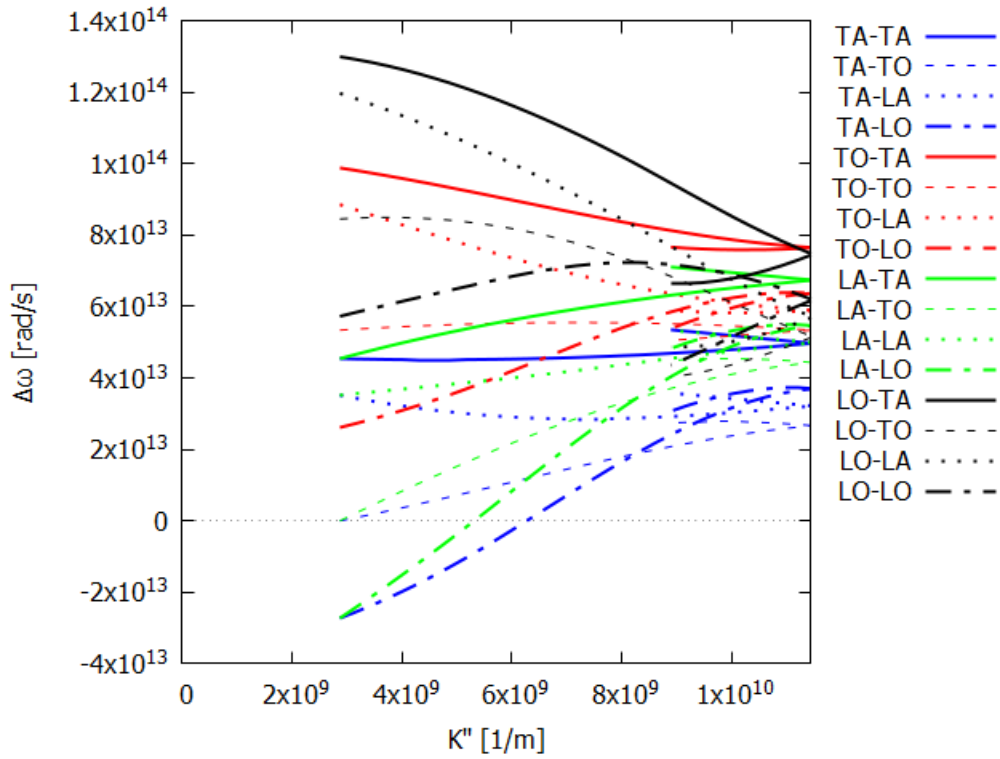


Figure 5: Scan results showing $\Delta\omega$ vs. K'' of a TO phonon at $K_{red} = \frac{1}{4}$

These figures show the complete scan of every branch combination, however, not every three-phonon combination can satisfy both the conservation equations. To make the combinations that satisfy conservation clearer, the following figures eliminate the combinations that cannot satisfy the conservation equations.

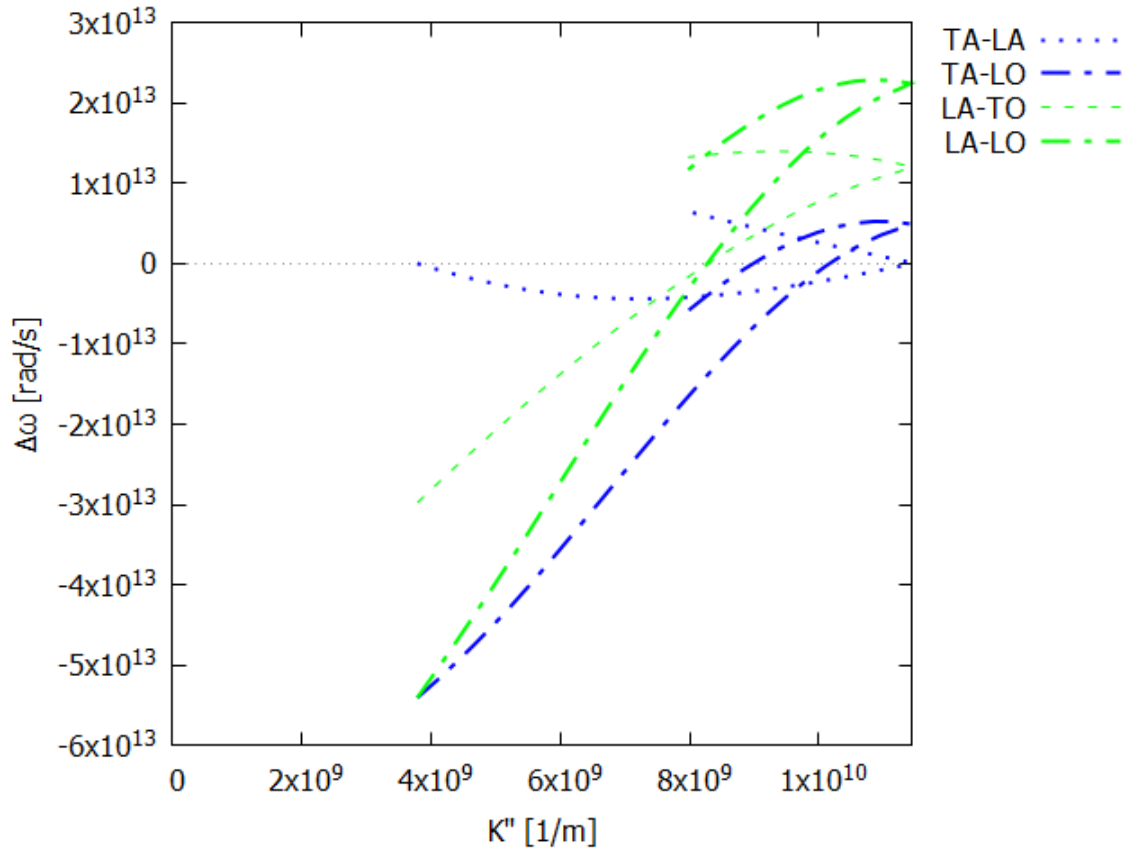


Figure 6: Scan results showing $\Delta\omega$ vs. K'' of an LA phonon at $K_{red} = \frac{1}{3}$ with the non-contributing combinations omitted

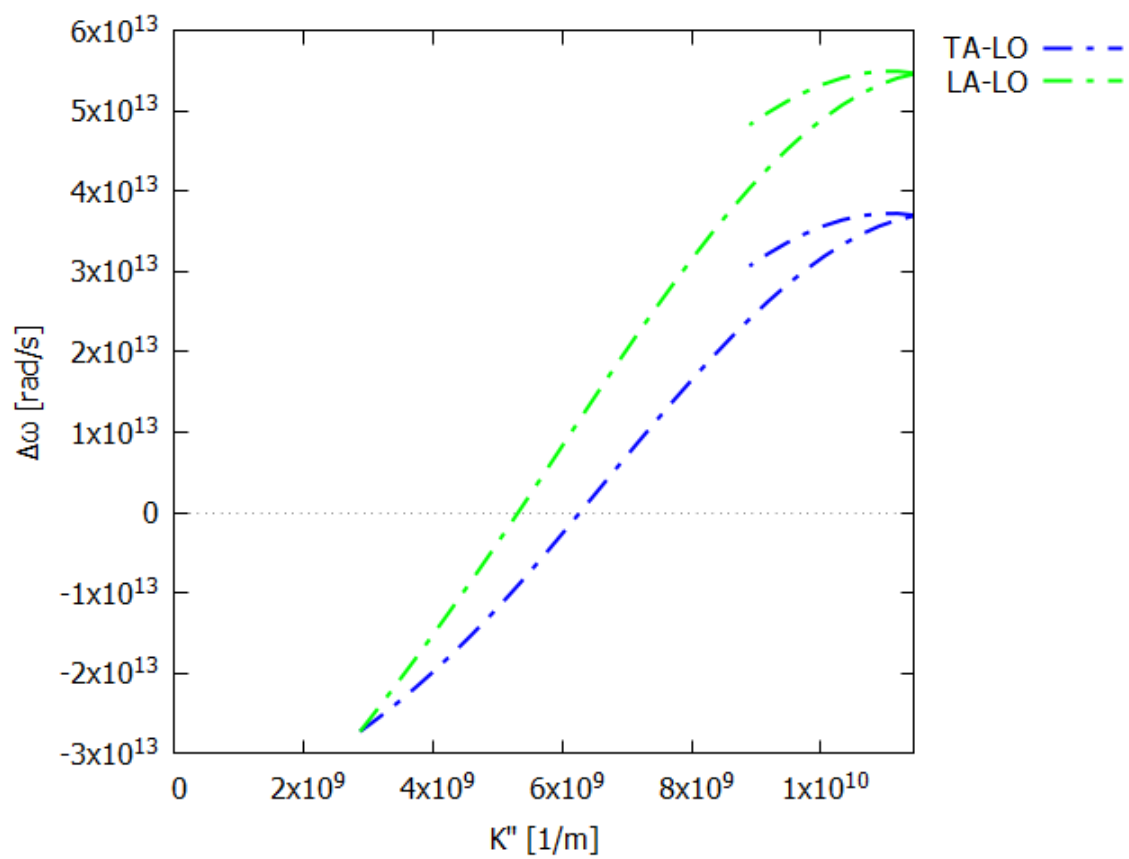


Figure 7: Scan results showing $\Delta\omega$ vs. K'' of a TO phonon at $K_{red} = \frac{1}{4}$ with the non-contributing combinations omitted

CALCULATION OF RELAXATION TIME

Relaxation time for a phonon is given by the equation [7].

$$\frac{1}{\tau_i} = \frac{\gamma^2 \hbar K'^2}{24\pi\rho v_{ph}^2 v_g'} \omega \omega' \omega'' [f_{K'}(\omega') - f_{K''}(\omega'')].$$

Where γ is the Grüneisen parameter which is set to 1.5. The Grüneisen parameter is used in other works as the only necessary fitting parameter for the relaxation time calculation [19]. \hbar is the reduced Plank's constant, ρ is the crystal density, v_{ph} is the phase velocity defined as ω/K . The frequencies $\omega \omega' \omega''$ correspond to each of the phonons in the three-phonon combination. The function $f_K(\omega)$ is the Bose-Einstein distribution function.

$$f_K(\omega) = \frac{1}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1}$$

Group velocity v_g is defined as $\delta\omega/\delta K$ and is shown in Figure 8. It also can be seen in Figure 1 that the longitudinal phonons have a larger group velocity because they have more variation in frequency as the wave vector changes.

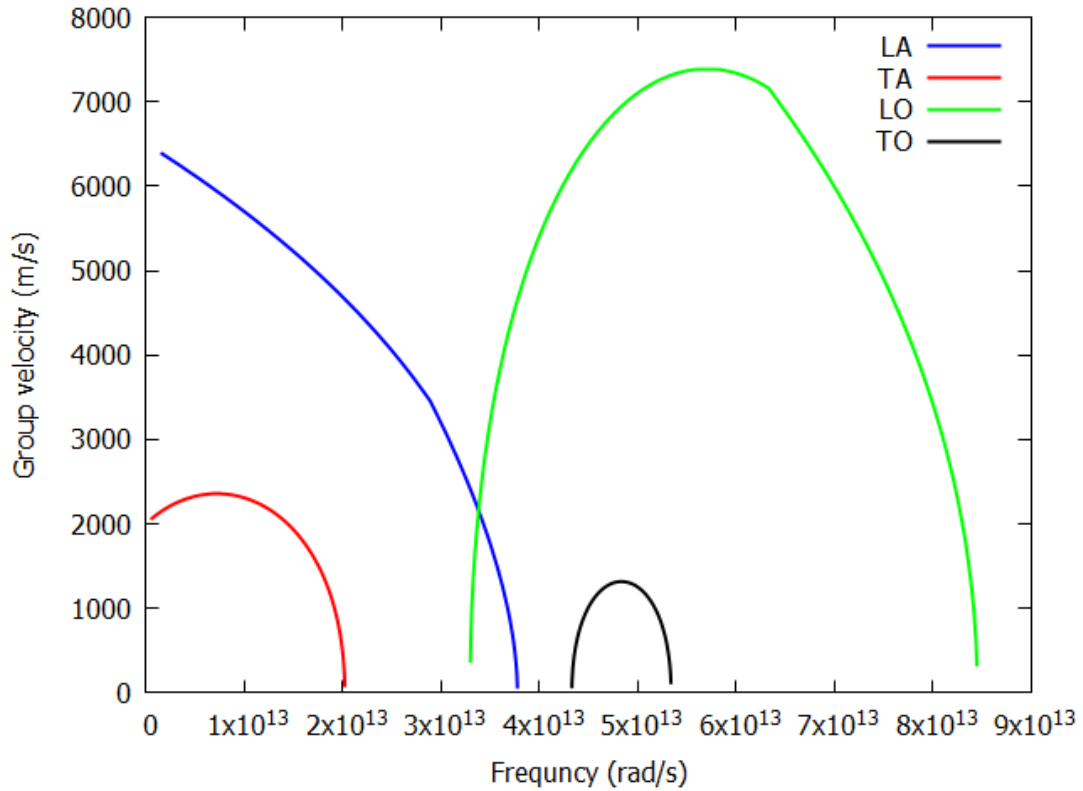


Figure 8: Group velocity for each of the 4 dispersion branches.

With a slight addition to the scan routine detailed above, the code can compute the relaxation time for each of the phonons as the scan is in progress. This is done by creating a loop outside the scan routine that will change the primary phonon wave vector and branch. The overall relaxation time is obtained through Mathiessen's rule which sums all the contributing relaxation times.

$$\frac{1}{\tau} = \sum_n \frac{1}{\tau_n}$$

When the scattering event becomes a U-process the equation for calculating relaxation time is modified slightly to become.

$$\frac{1}{\tau_i} = \frac{\gamma^2 \hbar K'^2}{24\pi\rho v_{ph}^2 v_g'} \omega\omega'\omega'' \left[\frac{1}{2} \{f_{K'}(\omega') + f_{K''}(\omega'') + 1\} \right].$$

Taking this into consideration, it is possible to isolate the relaxation time contribution from each of the two types of scattering which may be beneficial in future work.

However, with Mathiessen's rule the total relaxation time includes both N-process and U-process scattering.

RESULTS AND DISCUSSION

With each of the parts to the relaxation time equation in place the total relaxation time can be calculated at different temperatures. The figures below show the relaxation times of each phonon branch at 300K and 1000K.

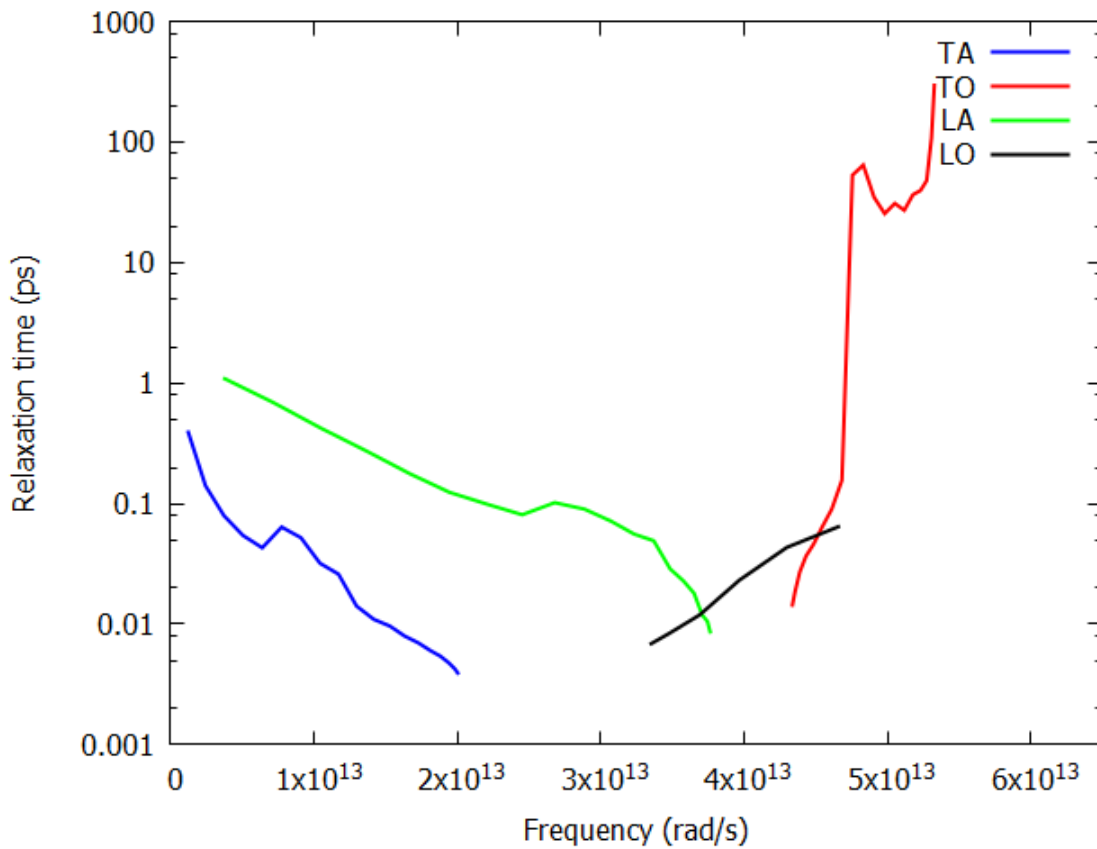


Figure 9: Relaxation time vs frequency of the phonon branches at 300K

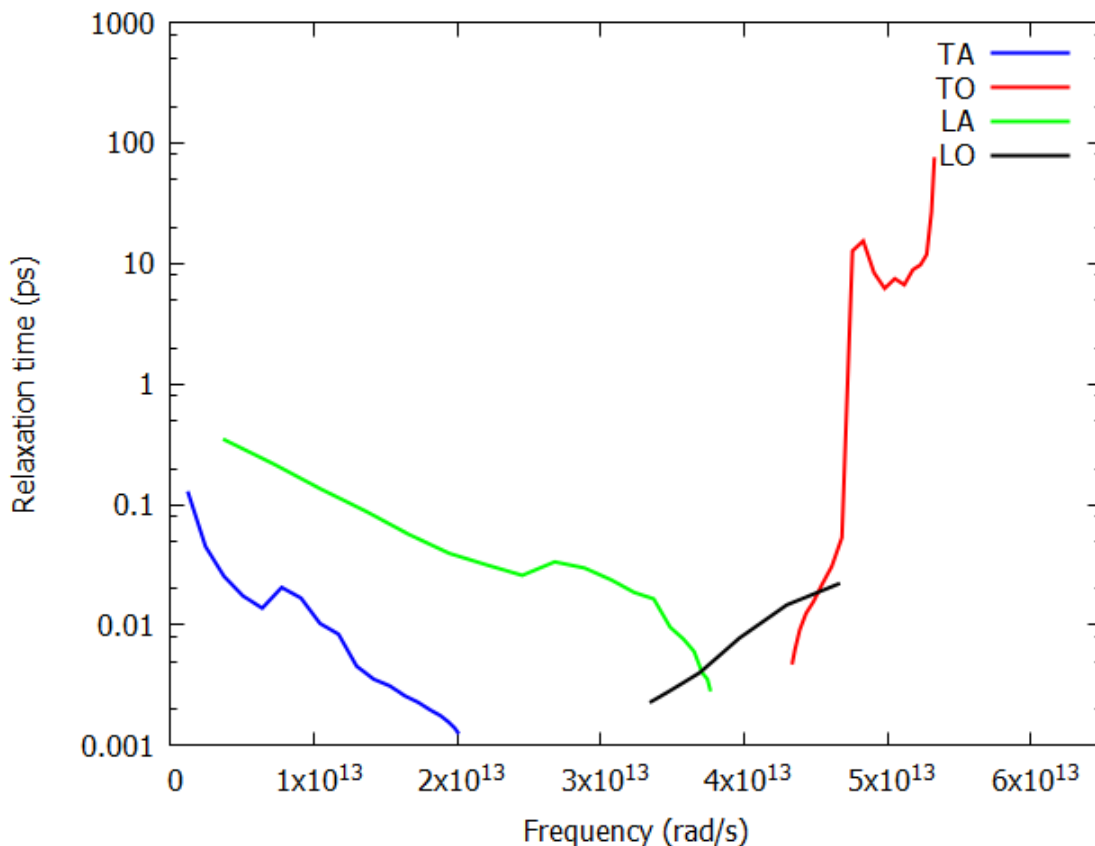


Figure 10: Relaxation time vs frequency of the phonon branches at 1000K

The relaxation time plots are comparable to the results obtained by Deskins [1] except for the longitudinal optical branch which cuts off near 5×10^{13} . This is likely because the routine in this paper neglects two higher frequency optical branches that are included in the routine performed by Deskins.

The relaxation times at both temperatures have the same general shape and behavior but there is a slight difference in location. The relaxation time at 300K is higher than the relaxation time at 1000K. This makes sense because UO_2 at 1000K will have a higher energy than UO_2 at 300K and the phonons move more quickly.

With the relaxation time results it is possible to achieve thermal conductivity predictions of UO₂ using a modified version of the Boltzmann equation which was mentioned in the introduction [2].

$$\kappa = \frac{4\pi}{3} \frac{1}{(2\pi)^3} \sum_p \int [v_{Kp}^2 \tau(K,p) C_{ph}(K,p) f(K,p)] dK$$

Where v_{Kp} is phonon velocity, τ is the relaxation time $f(K,p)$ is the Bose-Einstein distribution p is the polarization of the phonon K is the wavevector and C_{ph} is the specific heat given by,

$$C_{ph} = \frac{kx^2 e^x}{(e^x - 1)^2}$$

Where $x = \frac{\hbar\omega}{kT}$ and k is the Boltzmann constant.

SUMMARY AND CONCLUSION

Building upon previous studies of phonon scattering in silicon and UO_2 this work provides additional insight into the effect of optical phonons in the computation of relaxation time. Optical phonons become increasingly important in simulations of alloys and composite structures. Using the phonon dispersion branches, a scan identified all possible three-phonon combinations that satisfy conservation of momentum and energy. These combinations are then used along with other phonon properties, such as group velocity, to obtain an effective relaxation time which has applications in finding thermal conductivity as well as Monte Carlo simulations [9]. Relaxation time for each of the branches of UO_2 is presented in the previous section.

A simulation based study such as this one is valuable when physical experimentation to find thermal properties is expensive, difficult or hazardous. Simulations based on phonon scattering can provide an accurate baseline to compare physical results and provide insight toward experiment design.

This treatment of phonon-phonon interaction also provides a good method for including optical phonons in the Monte Carlo code created by Dr. Roberts. The existing Monte Carlo simulation is for silicon and only considers acoustic phonons. The higher energy optical modes may cause more U-process scattering, and in turn help correct the calculation of thermal conductivity which tends to be too high. This is assumed because U-process scattering lowers thermal conductivity but has not yet been proven.

This work has built on the existing work done to treat phonon behavior with the specific motivation to apply it toward Monte Carlo simulations of UO_2 . Future work includes applying the relaxation time to the Boltzmann equation to compute thermal

conductivity at equilibrium as well as developing a Monte Carlo simulation for UO_2 and other materials based on their specific dispersion curves.

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