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Computer Physics Communications ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Computer Physics Communications

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An accelerated algorithm for full band electron–phonon scattering rate computation☆

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ARTICLE INFO

Article history:
Received 2 February 2014
Accepted 9 August 2014
Available online xxxx

Keywords:
Electron phonon interaction
Full band scattering
Accelerated algorithm

ABSTRACT

Computing scattering rates of electrons and phonons stands at the core of studies of electron transport properties. In the high field regime, the interactions between all electron bands with all phonon bands need to be considered. This full band interaction implies a huge computational burden in calculating scattering rates. In this study, a new accelerated algorithm is presented for this task, which speeds up the computation by two orders of magnitude (100 times) and dramatically simplifies the coding. At the same time, it visually demonstrates the physical process of scattering more clearly.

Program summary

Program title: Scattering_band_by_band
Catalogue identifier: AEUH_v1_0
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEUH_v1_0.html
Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland
Licensing provisions: Standard CPC licence, http://cpc.cs.qub.ac.uk/licence/licence.html
No. of lines in distributed program, including test data, etc.: 22914
No. of bytes in distributed program, including test data, etc.: 5785964
Distribution format: tar.gz
Programming language: Matlab.
Computer: All.
Operating system: All.
RAM: Depends on problem, ∼kB to MB
Classification: 16.5.

Nature of problem:
Electron–phonon scattering is a fundamental problem in studying electron transport in condensed matters. There are situations where the scattering rates need to be updated frequently during a simulation, e.g. when hot phonon effects are considered. The speed of scattering calculation is very important in such cases.

Solution method:
In searching for possible scattering events, we propose here a band-by-band method, instead of the traditional point by point method. The whole calculation is parallelized in this sense and dramatically accelerated. Moreover, we proposed a representation method for all scattering mechanisms, which greatly simplified the coding task. Also, the additional animation part of this program demonstrates many insights into the scattering process.

Restrictions:
To use the code directly, electron band and phonon band should have the same mesh size. In other words, for each phonon band and electron band, they should have the same number of data points.

☆ This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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http://dx.doi.org/10.1016/j.cpc.2014.08.009

Additional comments:
If high speed is desired, it is best to turn off the animation function.

Running time:
Running time depends on the problem size. For the example used in this paper, it takes about 144 seconds by 1 CPU on Dell PowerEdge 610 (A dual quad core server with CPU frequency of 3.0 GHz).

1. Introduction

In studying electron transport, interactions between electrons and phonons are always the first topic to address [1–5]. As electron bands are obtained under the adiabatic approximation, however the crystal lattice is never static and always vibrates. For electronics operating at a temperature of at least around 300 K, the interaction with phonon has the most significant contribution to electron scattering. In the high field regime, an electron is accelerated to a high energy state and then it can interact with all phonon bands. Therefore, full band scattering calculation is a must [6].

To obtain a better representation of scattering mechanism, a denser discretization scheme of electron and phonon bands is always preferred. As more data points are used, the computation time increases dramatically as well. If this calculation were a one-time task, it would still be acceptable. However, there are situations where a scattering rate needs to be updated frequently during ensemble Monte Carlo (EMC) simulation processes. For example, the scattering rates should be calculated repeatedly when the accumulation of hot phonons is considered [7,8]. The calculation of scattering rates consumes such a long time that it makes such simulations practically unfeasible.

In this paper, a new accelerated algorithm is presented to solve this difficulty by reducing computational time. Compared to the conventional point by point algorithm [9], the proposed technique calculates the scattering rate through a band-by-band technique. As a result, the computation task is parallelized.

2. Model problem

The ideas demonstrated here are quite general and applicable to any electron–phonon interaction system. As an example, the scattering rates for (10, 10) single walled carbon nanotube (SWCNT) are computed.

Due to the quantization in the circumferential direction, electrons have 20 subbands, with each denoted by υ. Except for subband 0 and subband 10, all other subbands are double degenerated, as can be seen in Fig. 1. In this study, the first Brillouin zone (BZ) for each electron subband is discretized into 2000 data points. Similarly, phonons are also quantized into subbands with subband number μ, and each phonon subband has 2000 data points in the first BZ. Only LA and LO phonons are considered for scattering mechanisms, as they have more contribution to scattering rates than traverse phonons [10,11].

LA and LO phonons can be absorbed or emitted, as well as be forwardly scattered or backwardly scattered. Up to this point, 8 different scattering mechanisms are already present for interactions of an electron with a specific phonon of subband μ. Given 20 phonon subbands for (10, 10) SWCNT in this study, the number of all scattering mechanisms is 160. The selection rule is determined by conservation laws [12], i.e. the conservation of energy:

$$E(k, \upsilon) - E(k', \upsilon') = \pm E_p(q, \mu); \tag{1}$$

the conservation of longitudinal momentum:

$$\hbar k - \hbar k' = \pm \hbar q; \tag{2}$$

and the conservation of circumferential momentum:

$$\upsilon - \upsilon' = \pm \mu. \tag{3}$$

In order to calculate the scattering rates for (10,10) SWCNT point by point, at least four layers of for-loop are needed [9]. For example, the first layer of loop should go through each subband of electrons, while the second layer of loop should go through each electron state of a specific electron subband. Correspondingly, another two layers of for-loop are needed for phonons. Additionally one more layer may be present to consider all scattering mechanisms listed above, or it can be even written out explicitly. Obviously, such an algorithm is quite time consuming.

3. Algorithm description

Instead of the point by point algorithm described above, the new algorithm presented in this study focuses more on the physical picture of scattering. First, let us consider the interaction between a whole electron subband with a specific phonon. When this phonon has positive momentum and is absorbed, the whole band should be shifted upwards by the energy of this phonon and be shifted to the right direction by the momentum of this phonon. Such a graphical interpretation can be generalized for all other scattering mechanisms as a combination of forward/backward scattering with absorption/emission.

Second, according to the conservation of subband numbers, the final subband number is determined. For example, after the electron in subband $\upsilon = 2$ absorbs a phonon in subband $\mu = 4$, its final subband number will be $2 + 4 = 6$. Electron subband 6 will be called the target subband here. Although the whole electron subband is shifted after interacting with a phonon, only those electron states or points located on target electron subband imply a possible scattering. Only the intersecting points mean scattering. Graphically, this process is demonstrated in Fig. 1. As shown in Fig. 1, an extended zone scheme is used for electron bands. And due to the symmetries of both electron and phonon band structures, only the right-hand side is considered or only states with positive wave vectors are considered.

To carry out a practical computation following the graphical description of the scattering process and selection rule, a numerical implementation is demonstrated by taking forward scattering as an example. The flowchart is shown in Fig. 2.

The data of each original electron subband are put into a column vector before considering its' interaction with a specific whole phonon subband, either LA phonon or LO phonon. After interacting with a specific phonon, each electron in this subband will gain or lose the momentum and energy of this phonon. The resulting column vector is obtained by adding or subtracting phonon energy from the original data according to absorption or emission scattering. At the same time, the indices of each electron should also be updated according to forward or backward scattering. From the first phonon of with wave vector q_0 to the last phonon of q_{1000}, each of those 1000 phonons will generate a new column vector, which will then be assembled into a shifted matrix side by side. This paragraph is summarized in Table 1.

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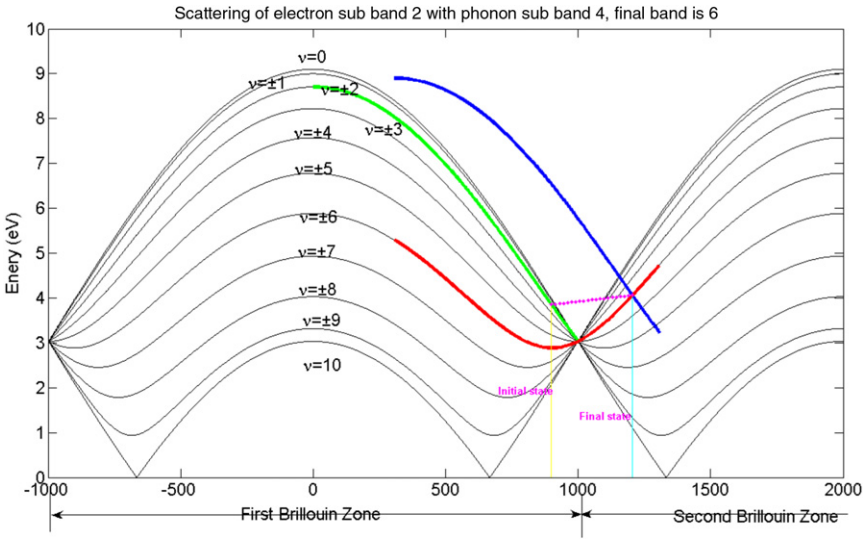

Fig. 1. Graphical representation of subband forward scattering, a forward LO phonon is absorbed. Black curves are electron subbands; the green curve is electron subband 2, to be scattered by phonon subband 4; the blue curve is shifted electron subband 2 after interacting with a phonon in subband 4; the red curve is the target electron subband 6, the subband number is determined by circumferential momentum conservation; the crossing point of blue and red curves implies a possible scattering; the dotted magenta line represents the jump of electron from the initial state to the final state. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 1
The shifted matrix for a forward absorption scattering k_i is wave vector of electrons; q_i are wave vector of phonons.

	q_1	q_2	...	q_{1000}
k_1	$E(k_1+q_1)+E_{ph}(q_1)$	$E(k_1+q_2)+E_{ph}(q_2)$	...	$E(k_1+q_{1000})+E_{ph}(q_{1000})$
k_2	$E(k_2+q_1)+E_{ph}(q_1)$	$E(k_2+q_1)+E_{ph}(q_2)$	...	$E(k_2+q_{1000})+E_{ph}(q_{1000})$
...	...	...	...	...
k_{999}	$E(k_{999}+q_1)+E_{ph}(q_1)$	$E(k_{999}+q_2)+E_{ph}(q_2)$	...	$E(k_{999}+q_{1000})+E_{ph}(q_{1000})$
k_{1000}	$E(k_{1000}+q_1)+E_{ph}(q_1)$	$E(k_{1000}+q_2)+E_{ph}(q_2)$	...	$E(k_{1000}+q_{1000})+E_{ph}(q_{1000})$

Table 2
Scattering mechanism by 4 bits binary number.

1st phonon		2nd energy		3rd momentum		4th subband	
0	1	0	1	0	1	0	1
LA	LO	Absorption	Emission	Forward	Backward	Forward	Backward

For each column shown in Table 1, their indices are monotonically either increasing (forward scattering) or decreasing (backward scattering). A similar targeted matrix can be obtained from the targeted electron subband, which is decided by the conservation of subband numbers. While the first column is just the subband in the first Brillouin zone, following columns are obtained from the same subband by moving this interval to right or left according to forward or backward scattering. The resulting matrix is named shifted matrix.

With both shifted matrix and targeted matrix at hand, the next step is to pick out the possible scatterings. In the graphical representation, scattering happens wherever a cross presents. Numerically, crossing points can be found by studying the difference between shifted and targeted matrices. Column by column, the difference means the distance between the shifted subband curve and the targeted subband curve. The crossing points always occur where the sign of difference changes. For these large matrices of the dimension of 1000 by 1000, the possible scattering is usually on the order of hundreds. Therefore, the task of calculating scattering rates using the method of band by band shrinks roughly about 1000 times, compared with the point by point method.

The last challenge is to lump all possible scattering mechanisms into one loop. For each scattering events, a four step choice needs to be made: (a) LA or LO; (b) emission or absorption; (c) forward or backward; (d) subband forward or subband backward. Since each step has only two choices, a specific scattering mechanism can be represented by 4 bits binary number, as shown in Table 2. Each bit stands for the selection of the above four step choice.

This representation of scattering mechanism is not only a convenience in notation, but also has a mathematical meaning. Besides determining whether an electron interacts with LA phonon or LO phonon, other choices in electron scattering with phonon are just about plus or minus between physical parameters of electron and phonon. And $\pm$ can be easily expressed by (-1)^bit, which results $+$ for bit $= 0$ while $-$ for bit $= 1$.

To make it more clear, the final energy after electron scatting is $E\left(k', v'\right) = E(k, v) + (-1)^{\text{bit}(2)} E_{ph}(q, \mu)$. Similarly, the final wave number is $k' = k + (-1)^{\text{bit}(3)} q$ and final subband is $v' = v + (-1)^{\text{bit}(4)} \mu$. For example, (0 1 1 0) means that the scattering emits an LA phonon with longitudinal backward scattering while the subband forwards scattering. In the decimal system, these 4 bits binary numbers will be 0–15. With this technique, all different scattering mechanisms can have the same formula in programming. It dramatically simplifies the coding, as well.

4. Results and discussions

Based on the previous discussion, a program is written and implemented. The entire calculation of scattering rate for (10, 10) SWCNT takes 144 s on 1 CPU of Dell PowerEdge 610 (a dual quad core server with CPU frequency of 3.0 GHz). For comparison, an existing program written in the point by point method takes up to 136 min [9]. We should also point out that in the band-by-band calculation, both electron and phonon subbands have 1000 data points for half of the first BZ, while the later (traditional point by point code) has only 500 data points for phonon subbands. With an

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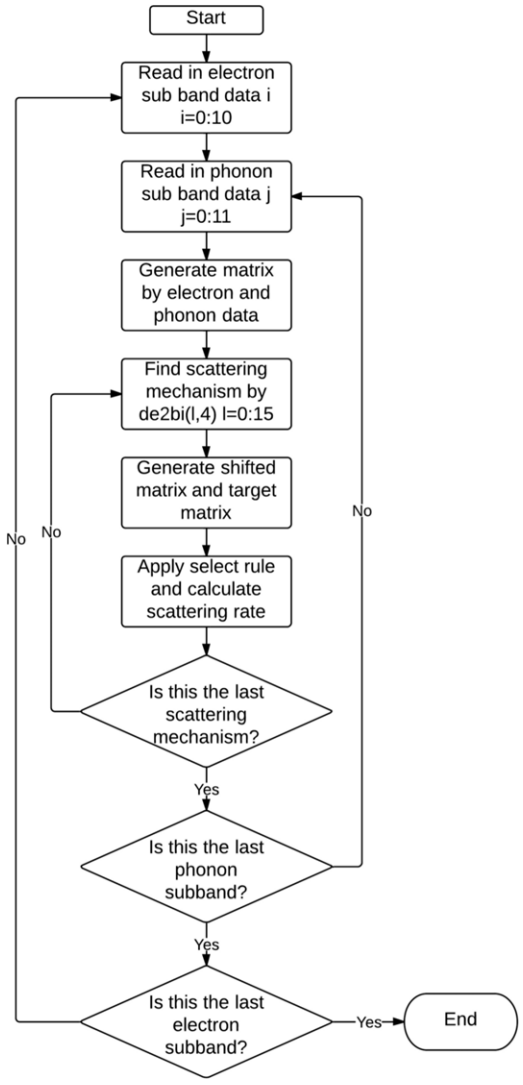

Fig. 2. Flow chart of the band-by-band scattering algorithm.

ideal assumption that the computation load only increase linearly following the size of the problem, the first program has finished four times more calculations. Or for the same size problem, the first program will only take about 72 s, which is 1.2 min. Therefore, the new program runs more than 100 times faster than the conventional point by point scattering program.

Of course, accuracy of the results is much more important than speed. Since most electrons in SWCNT reside in electron subband 10 and subband 9, only scattering rates of those two subbands are presented here. But the comparison has been done for all the subbands, although not shown here.

Scattering rates of electron subband 9 and subband 10 by phonons are shown in Figs. 3–6. Green curves are results obtained by [9] (point by point algorithm), while red stars are results obtained by the band-by-band algorithm. Both algorithms give results on the same order of magnitude and have similar behavior. But it is obvious that the band-by-band algorithm always gives slightly larger scattering values. Since all these results are plotted in a semi-log format, the higher values of red stars are at least 2 times larger than corresponding data points on green curves. Such big differences should be explained or justified.

After scrutinizing these two programs, it turns out that the point by point program [9] has some deficiency. It presumes that when an electron state interacts with a phonon subband, the electron can only be scattered by at most one phonon of this subband. This assumption is alluring and unquestionable at first thought as it can speed up the calculation by exiting the loop through a phonon subband whenever a scattering is found. But with the help of graphical animation of band-by-band program, we found that the previous assumption is insufficient. Significant improvements can be obtained by simply removing those premature exit mechanisms in looping through phonon subbands. Results of the improved point by point program are demonstrated in Figs. 3–6 as blue curves.

5. Conclusions

The proposed band-by-band algorithm for scattering rate computation dramatically speeds up the calculation. According to the test, the band-by-band algorithm runs about 100 times faster than the point by point algorithm. The acceleration mainly comes from parallelization, instead of five layers for-loop in the conventional algorithm here only two are given. At the same time, the band-by-band algorithm also provides a much clearer physical picture. In addition, the binary representation of scattering mechanisms greatly simplifies the coding task.

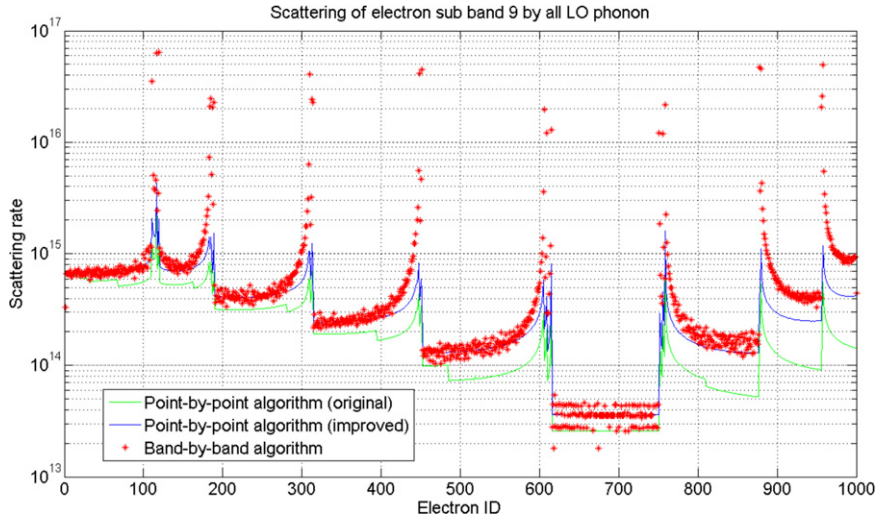

Fig. 3. Scattering rates of electron subband 9 by LO phonons. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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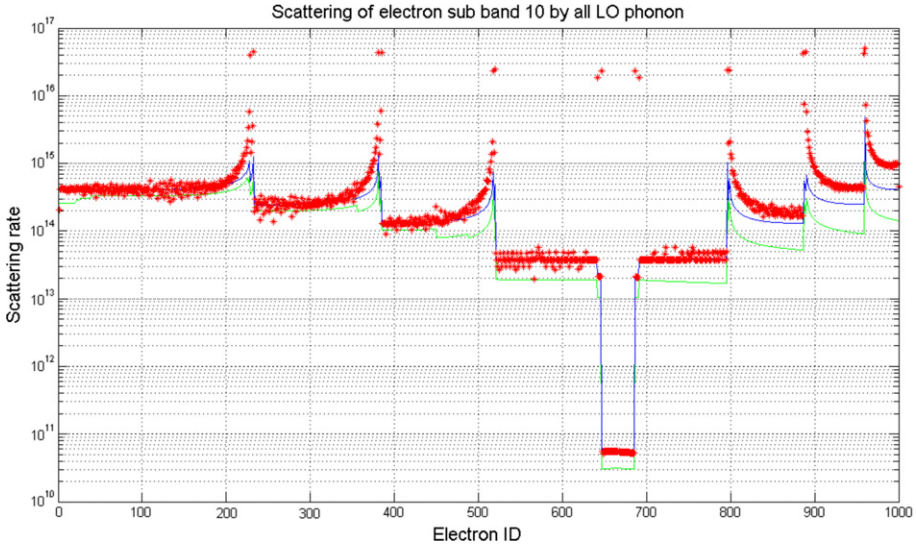

Fig. 4. Scattering rates of electron subband 10 by LO phonons. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

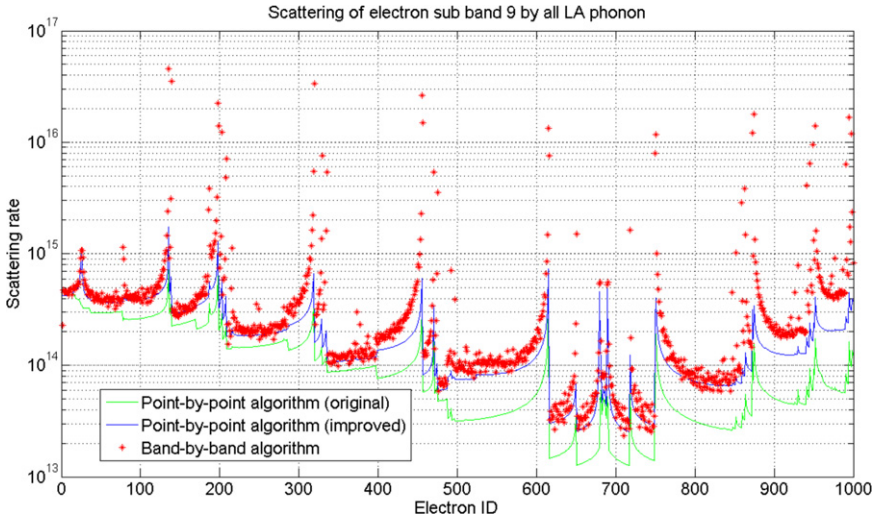

Fig. 5. Scattering rates of electron subband 9 by LA phonons. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

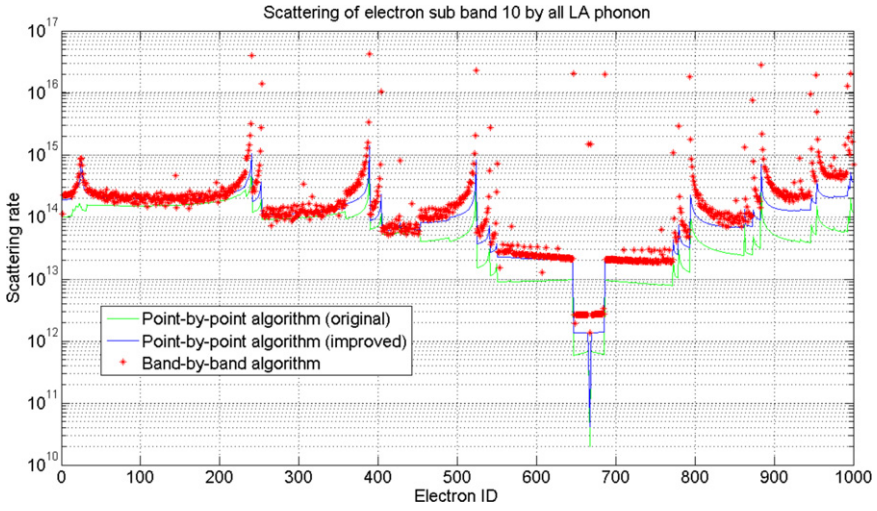

Fig. 6. Scattering rates of electron subband 10 by LA phonons. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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Acknowledgment

This project has been funded by the US Navy office of Naval Research Advanced Electrical Power Systems (N00014-11-1-0543) under the direction of Dr. Peter Chu.

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