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Submit only ONE copy of this form **for each PI/PD and co-PI/PD** identified on the proposal. The form(s) should be attached to the original proposal as specified in GPG Section II.C.a. Submission of this information is voluntary and is not a precondition of award. This information will not be disclosed to external peer reviewers. ***DO NOT INCLUDE THIS FORM WITH ANY OF THE OTHER COPIES OF YOUR PROPOSAL AS THIS MAY COMPROMISE THE CONFIDENTIALITY OF THE INFORMATION.***

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Ethnicity: (Choose one response) ☐ Hispanic or Latino ☒ Not Hispanic or Latino

Race: (Select one or more)
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- ☐ Asian
- ☐ Black or African American
- ☐ Native Hawaiian or Other Pacific Islander
- ☒ White

Disability Status: (Select one or more)
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- ☐ Visual Impairment
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Race Definitions:
American Indian or Alaska Native. A person having origins in any of the original peoples of North and South America (including Central America), and who maintains tribal affiliation or community attachment.
Asian. A person having origins in any of the original peoples of the Far East, Southeast Asia, or the Indian subcontinent including, for example, Cambodia, China, India, Japan, Korea, Malaysia, Pakistan, the Philippine Islands, Thailand, and Vietnam.
Black or African American. A person having origins in any of the black racial groups of Africa.
Native Hawaiian or Other Pacific Islander. A person having origins in any of the original peoples of Hawaii, Guam, Samoa, or other Pacific Islands.
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PI/PD Name: Yang Wang

Gender: ☒ Male ☐ Female

Ethnicity: (Choose one response) ☐ Hispanic or Latino ☒ Not Hispanic or Latino

Race: (Select one or more)
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- ☐ Native Hawaiian or Other Pacific Islander
- ☐ White

Disability Status: (Select one or more)
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List of Suggested Reviewers or Reviewers Not To Include (optional)

SUGGESTED REVIEWERS:
Not Listed

REVIEWERS NOT TO INCLUDE:
Not Listed

COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

PROGRAM ANNOUNCEMENT/SOLICITATION NO./CLOSING DATE/if not in response to a program announcement/solicitation enter NSF 09-29

PD 09-1765 **10/31/09**

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☐ IF THIS IS A PRELIMINARY PROPOSAL THEN CHECK HERE

TITLE OF PROPOSED PROJECT **Phonon Transport Near and Across Seminductor Interfaces**

REQUESTED AMOUNT	PROPOSED DURATION (1-60 MONTHS)	REQUESTED STARTING DATE	SHOW RELATED PRELIMINARY PROPOSAL NO. IF APPLICABLE
$ **353,355**	**36** months	**09/01/10**	

CHECK APPROPRIATE BOX(ES) IF THIS PROPOSAL INCLUDES ANY OF THE ITEMS LISTED BELOW

☐ BEGINNING INVESTIGATOR (GPG I.G.2)
☐ DISCLOSURE OF LOBBYING ACTIVITIES (GPG II.C.1.e)
☐ PROPRIETARY & PRIVILEGED INFORMATION (GPG I.D, II.C.1.d)
☐ HISTORIC PLACES (GPG II.C.2.j)
☐ EAGER* (GPG II.D.2) ☐ RAPID** (GPG II.D.1)
☐ VERTEBRATE ANIMALS (GPG II.D.6) IACUC App. Date _____
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PI/PD DEPARTMENT
Mechanical Engineering

PI/PD FAX NUMBER
412-268-3348

PI/PD POSTAL ADDRESS
5000 FORBES AVE
SH 310
PITTSBURGH, PA 152133890
United States

NAMES (TYPED)	High Degree	Yr of Degree	Telephone Number	Electronic Mail Address
PI/PD NAME **Alan McGaughey**	**PhD**	**2004**	**412-268-9605**	**mcgaughey@cmu.edu**
CO-PI/PD **Yang Wang**	**PhD**	**1993**	**412-268-2795**	**ywg@psc.edu**
CO-PI/PD				
CO-PI/PD				
CO-PI/PD				

CERTIFICATION PAGE

Certification for Authorized Organizational Representative or Individual Applicant:

By signing and submitting this proposal, the Authorized Organizational Representative or Individual Applicant is: (1) certifying that statements made herein are true and complete to the best of his/her knowledge; and (2) agreeing to accept the obligation to comply with NSF award terms and conditions if an award is made as a result of this application. Further, the applicant is hereby providing certifications regarding debarment and suspension, drug-free workplace, and lobbying activities (see below), nondiscrimination, and flood hazard insurance (when applicable) as set forth in the NSF Proposal & Award Policies & Procedures Guide, Part I: the Grant Proposal Guide (GPG) (NSF 09-29). Willful provision of false information in this application and its supporting documents or in reports required under an ensuing award is a criminal offense (U. S. Code, Title 18, Section 1001).

Conflict of Interest Certification

In addition, if the applicant institution employs more than fifty persons, by electronically signing the NSF Proposal Cover Sheet, the Authorized Organizational Representative of the applicant institution is certifying that the institution has implemented a written and enforced conflict of interest policy that is consistent with the provisions of the NSF Proposal & Award Policies & Procedures Guide, Part II, Award & Administration Guide (AAG) Chapter IV.A; that to the best of his/her knowledge, all financial disclosures required by that conflict of interest policy have been made; and that all identified conflicts of interest will have been satisfactorily managed, reduced or eliminated prior to the institution's expenditure of any funds under the award, in accordance with the institution's conflict of interest policy. Conflicts which cannot be satisfactorily managed, reduced or eliminated must be dislosed to NSF.

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By electronically signing the NSF Proposal Cover Sheet, the Authorized Organizational Representative or Individual Applicant is providing the Drug Free Work Place Certification contained in Exhibit II-3 of the Grant Proposal Guide.

Debarment and Suspension Certification

(If answer "yes", please provide explanation.)

Is the organization or its principals presently debarred, suspended, proposed for debarment, declared ineligible, or voluntarily excluded from covered transactions by any Federal department or agency? Yes ☐ No ☒

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The following certification is required for an award of a Federal contract, grant, or cooperative agreement exceeding $100,000 and for an award of a Federal loan or a commitment providing for the United States to insure or guarantee a loan exceeding $150,000.

Certification for Contracts, Grants, Loans and Cooperative Agreements

The undersigned certifies, to the best of his or her knowledge and belief, that:

(1) No federal appropriated funds have been paid or will be paid, by or on behalf of the undersigned, to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any federal contract, the making of any Federal grant, the making of any Federal loan, the entering into of any cooperative agreement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.

(2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit Standard Form-LLL, ''Disclosure of Lobbying Activities,'' in accordance with its instructions.

(3) The undersigned shall require that the language of this certification be included in the award documents for all subawards at all tiers including subcontracts, subgrants, and contracts under grants, loans, and cooperative agreements and that all subrecipients shall certify and disclose accordingly.

This certification is a material representation of fact upon which reliance was placed when this transaction was made or entered into. Submission of this certification is a prerequisite for making or entering into this transaction imposed by section 1352, Title 31, U.S. Code. Any person who fails to file the required certification shall be subject to a civil penalty of not less than $10,000 and not more than $100,000 for each such failure.

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Two sections of the National Flood Insurance Act of 1968 (42 USC §4012a and §4106) bar Federal agencies from giving financial assistance for acquisition or construction purposes in any area identified by the Federal Emergency Management Agency (FEMA) as having special flood hazards unless the:

(1) community in which that area is located participates in the national flood insurance program; and
(2) building (and any related equipment) is covered by adequate flood insurance.

By electronically signing the NSF Proposal Cover Sheet, the Authorized Organizational Representative or Individual Applicant located in FEMA-designated special flood hazard areas is certifying that adequate flood insurance has been or will be obtained in the following situations:

(1) for NSF grants for the construction of a building or facility, regardless of the dollar amount of the grant; and
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AUTHORIZED ORGANIZATIONAL REPRESENTATIVE	SIGNATURE	DATE
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* EAGER - EArly-concept Grants for Exploratory Research
** RAPID - Grants for Rapid Response Research

Phonon Transport Near and Across Semiconductor Interfaces

Alan McGaughey, Carnegie Mellon University & Yang Wang, Pittsburgh Supercomputing Center

Project Summary

The objective of the proposed work is to identify and understand the mechanisms of phonon transport near and across interfaces in nanostructured materials. Atomistic modeling tools [lattice dynamics calculations, the Boltzmann transport equation, molecular dynamics simulation, and density functional theory (DFT) calculations] and theoretical development will be applied to address fundamental questions regarding phonon propagation and scattering under conditions very different from what exists in a bulk phase.

Previous modeling work has focused on perfect, isolated interfaces described by simplified models or empirical interatomic potentials. Applying the results of such investigations to realistic systems, where the interfaces are imperfect, strained, and closely spaced, is questionable. Existing experimental techniques are limited to isolated interfaces where one of the species is a metal and to limited probing of individual phonons.

Intellectual Merit

The intellectual merit of the proposed work will be found in (i) an improved atomistic foundation for understanding interfacial phonon transport, and (ii) a suite of computational tools for studying phonon transport near and across interfaces at a level of accuracy and detail that is not currently available. Specifically, I will:

- Derive an expression for the phonon-interface scattering rate.
- Resolve the discrepancies between different thermal boundary resistance models by predicting the non-equilibrium phonon distributions that exist at interfaces.
- Demonstrate that DFT calculations can be used to provide the input for lattice-dynamics based thermal boundary resistance models. Use the DFT-based predictions to assess the role of electrons in thermal transport across metal-semiconductor interfaces.
- Identify how Bloch phonon modes develop as you move from an isolated interface to multiple interfaces to a periodic superlattice.
- Probe the role of interfacial species mixing in phonon transport across interfaces.

Broader Impact

The proposed work will broadly impact the wealth of technologically important systems that contain multi-layer components (e.g., the SiO_2 layer in a field-effect transistor, $Si/Si_{1-x}Ge_x$ and Bi_2Te_3/Sb_2Te_3 superlattices for thermoelectric energy conversion applications, and quantum cascade lasers and light emitting diodes built from layers of GaAs, AlGaAs, and GaN). The analysis tools will be suitable for studying any material system where phonons are the dominant thermal energy carriers.

The application of electronic structure calculations for predicting thermal transport properties is exciting. Few researchers are currently exploring this approach, in large part because of the theoretical and computational complexity. My extensive experience in working with atomistic computational tools places me in a unique position to take on this challenging and important research opportunity.

This project will also promote education and advance research in the emerging field of heat transfer physics: the study of thermal transport at the carrier-level (i.e., phonons, photons, electrons, and fluid particles). NanoHUB and thermalHUB, two online resources, will be used to disseminate general information and research findings. Discovery-based lectures will be developed and presented in undergraduate classes and through Pittsburgh-based outreach programs.

TABLE OF CONTENTS

For font size and page formatting specifications, see GPG section II.B.2.

*Proposers may select any numbering mechanism for the proposal. The entire proposal however, must be paginated. Complete both columns only if the proposal is numbered consecutively.

Project Description

1 Introduction

1.1 Motivation

The objective of the proposed work is to identify and understand the mechanisms of phonon transport near and across interfaces in nanostructured materials. Atomistic modeling and theoretical development will be applied to address fundamental questions regarding phonon propagation and scattering under conditions different from what exists in a bulk phase.

Materials with characteristic dimensions on the order of nanometers (i.e., nanostructured materials) have found application in the semiconductor and energy industries, where the small length scales and closely-spaced interfaces allow for the independent control of electrons and phonons.[1–6] For example, the width and composition of $Si_{1-x}Ge_x$ layers in electronic and optoelectronic devices (e.g., IBM and AMD's 45 nm process node transistor technology[7]) can be tuned to control their electronic band structure.[8–12] The active region in a quantum cascade laser or a light-emitting diode contains 1-10 nm thick films of direct bandgap semiconductors such as GaAs, AlGaAs, and GaN.[13,14] $Si/Si_{1-x}Ge_x$ superlattices and $Si_{1-x}Ge_x$ nanostructured materials are promising candidates for thermoelectric energy conversion (see Fig. 1).[15–24]

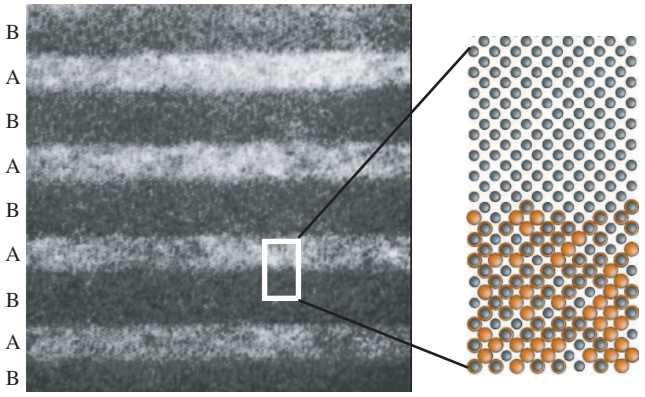

Figure 1: Epitaxially-grown $Si/Si_{0.78}Ge_{0.22}$ superlattice[5] and a representation of the atomic structure at an internal interface.

Significant experimental and theoretical challenges exist related to understanding how phonons interact with interfaces.[25,26] As such, despite over five decades of research, a robust model for the thermal boundary resistance has remained elusive.[27–29] Experimental techniques exist for measuring the thermal boundary resistance of a single, isolated interface where one of the materials is a metal.[30–33] It is not currently possible to measure the thermal boundary resistance of a semiconductor-semiconductor interface or resolve the contributions of the individual interfaces in a multi-layer system. Methods also exist for characterizing individual phonon modes in superlattices,[34–36] but are limited to long-wavelength acoustic modes. Thus, such approaches cannot offer insight into the dynamics of the full phonon spectrum, required for an accurate description of phonon scattering processes. Phonon transport near and across isolated interfaces has been characterized using continuum-level models,[27,28,37] lattice dynamics calculations,[38–44] and molecular dynamics (MD) simulations.[44–50] Outside of investigating superlattices, where the focus has been on thermal conductivity prediction,[51–62] few studies have considered the more general problem of closely spaced interfaces[40,63–65] and how they might be used to control phonon transport.

1.2 Fundamental Questions and Research Contribution

Fundamental questions remain regarding phonon transport near and across interfaces:

- Different theoretical/modeling approaches predict different thermal boundary resistances for the same interface. Can these different predictions be resolved?

- What are the contributions of inelastic phonon scattering and electrons, which are neglected in the majority of thermal boundary resistance models?
- At what point does an increasing number of closely spaced interfaces lead to the formation of coherent Bloch modes?
- What role do the confining species play on phonon transport in a thin film?

I propose to address these questions by using lattice dynamics calculations, the Boltzmann transport equation (BTE), Landauer theory, and MD simulation to study model systems with the diamond structure described by the Stillinger-Weber (SW) potential.[66–68] Realistic models of semiconductor/semiconductor and semiconductor/metal interfaces will then be considered using input from density functional theory (DFT) calculations. The DFT-based predictions will be compared to experimental data. In addressing the above questions, I will:

- Derive an expression for the phonon-interface scattering rate.
- Predict the non-equilibrium phonon distribution functions on either side of an interface.
- Assess the contribution of electrons to thermal transport across metal/nonmetal interfaces.
- Demonstrate the phonon mode-dependent transition from incoherent to coherent phonon transport (i.e., the formation of Bloch modes) in multi-layer structures.

1.3 Intellectual Merit and Broader Impact

The intellectual merit of the proposed work will be found in the innovative ways that lattice dynamics calculations, the BTE, MD simulation, and DFT will be applied to study interfacial phonon transport. I will predict quantities inaccessible in experiments or current modeling capabilities (e.g., the thermal boundary resistance of closely spaced interfaces) that will help to guide future modeling and experimental efforts. The methodologies developed will be applicable to studies of phonon transport in any system where atomic vibration is the dominant energy transfer mechanism.

By helping experimentalists to design nanostructured materials with tailored thermal transport properties, the proposed work will broadly impact systems where interfaces are critical (e.g., field effect transistors, heterojunction bipolar transistors, semiconductor lasers, light emitting diodes, thermoelectric materials). This work will also contribute to the growing discipline of materials design through computer simulation. The National Science Foundation Blue Ribbon Panel on Simulation Based Engineering Science wrote:[69]

> "With the depth of its intellectual development and its wide range of applications, computer simulation has emerged as a powerful tool, one that promises to revolutionize the way engineering and science are conducted in the twenty-first century."

The proposed work fits directly into this exciting and important field.

1.4 Synergistic Educational Activities

In parallel with the research endeavors, I will coordinate educational activities to generate interest and create community in heat transfer physics (the study of thermal transport at the carrier level) among students and researchers at Carnegie Mellon University (CMU) and worldwide. I will contribute research and educational materials to nanoHUB[70] and thermalHUB,[71] two NSF-sponsored websites whose mission is to serve the global nanotechnology and heat transfer communities. I will also incorporate heat transfer physics into the mechanical engineering curriculum at CMU. This objective will be accomplished by developing lectures for existing core courses and through a new course in heat transfer physics. The lectures will be adapted for high school students and delivered through Pittsburgh-based outreach programs.

1.5 PI Background and Qualifications

Over the last nine years, I have worked on a broad range of problems related to modeling thermal transport at the nanoscale, placing me in an ideal position to carry out the proposed research. I have used a variety of MD- and lattice dynamics-based techniques to study thermal transport in bulk materials[72–80] and nanostructures,[44,60–62,65,79,81–83] with a focus on understanding how atomic structure, phonon properties, and system-level thermal transport are related. Recent work has focused on silicon- and germanium-based materials from both top-down (thermal conductivity prediction)[62,78] and bottom-up (thermal boundary resistance prediction)[44,65] approaches. I have also made significant progress in the development, implementation, and refinement of anharmonic lattice dynamics methods for predicting phonon properties and thermal conductivity.[77–79,81,83,84] My research group has developed computer codes suitable as starting points for many of the proposed tasks. The computer hardware required to carry out the simulations/calculations is available in my research group (see the Facilities, Equipment, and Other Resources section) and at the NSF-sponsored Pittsburgh Supercomputing Center, where I have a development grant. I have developed and taught graduate courses in molecular simulation and heat transfer physics and am committed to exposing students and researchers to these fields.

Co-PI Wang will support the DFT calculations. He is a Senior Computational Scientist at the Pittsburgh Supercomputing Center (a ten minute walk from CMU) and is an expert in linear-scaling DFT techniques for massively-parallel high-performance computing environments.[85–91]

2 Thermal Boundary Resistance Prediction

Consider thermal transport by phonons across a junction between two semi-infinite leads, as shown in Fig. 2(a). The thermal resistance of the junction, R, is defined as

$$R = \frac{T_L - T_R}{q}, \tag{1}$$

where q is the heat flux across it and T_L and T_R are the temperatures at the lead/junction boundaries. If the junction contains a single interface [see Fig. 2(b)] and the phonon scattering within the junction is purely elastic (i.e., no inelastic phonon-phonon scattering), the thermal boundary resistance is equal to the thermal resistance of the junction.

An accurate prediction of thermal boundary resistance requires a detailed atomistic treatment.* Molecular dynamics simulations can be used to predict the thermal boundary resistance through a direct application of Eq. (1).[44,45,48–50,55,92–94] While straightforward to implement, this so called "direct method" approach requires significant computation time, is classical in nature, and does not provide detailed information about the phonon transport.

An expression for the thermal boundary resistance can be developed using the properties of the phonons in the system. Each lead emits phonons to and absorbs phonons from the junction. At steady-state, the net heat flux across the junction, q, is

$$q = \frac{1}{8\pi^3}\left[\int_L \sum_\nu^{+} \hbar\omega v_z(\boldsymbol{\kappa},\nu)\alpha_{LR}(\boldsymbol{\kappa},\nu)f_L(\boldsymbol{\kappa},\nu)d\boldsymbol{\kappa} + \int_R \sum_\nu^{-} \hbar\omega v_z(\boldsymbol{\kappa},\nu)\alpha_{RL}(\boldsymbol{\kappa},\nu)f_R(\boldsymbol{\kappa},\nu)d\boldsymbol{\kappa}\right], \tag{2}$$

where L and R denote the left and right leads, $\hbar$ is the Planck constant divided by 2π, ν denotes the phonon polarization, and $\boldsymbol{\kappa}$, ω, and v_z are the phonon wavevector, frequency, and component

*The commonly-used acoustic and diffuse mismatch models[28,37] for predicting thermal boundary resistance require a specification of the degree of diffuse scattering and use bulk properties for input (i.e., they do not consider the structure of the interface). The predictions of neither model agrees with experimental data above temperatures of 30 K. They are thus not suitable for the proposed work, where the objective is to accurately characterize phonon transport at typical device operating temperatures and to relate the findings to the atomic structure.

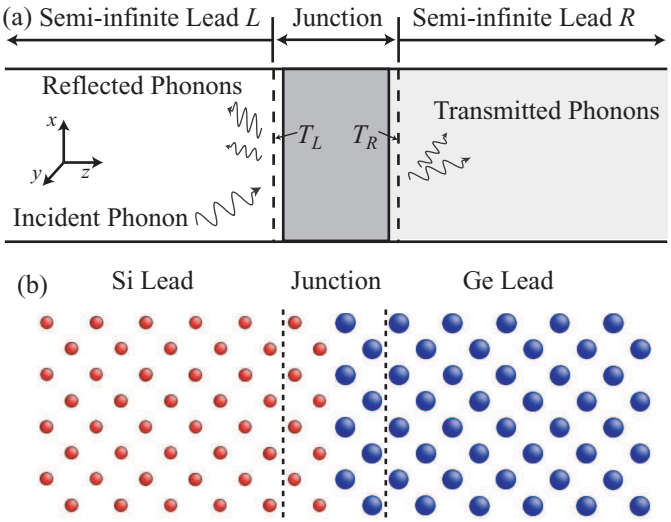

Figure 2: (a) Schematic diagram of lead/junction/lead system. The junction may contain one interface or multiple interfaces. (b) Setup for scattering boundary method calculations on an isolated Si/Ge interface.

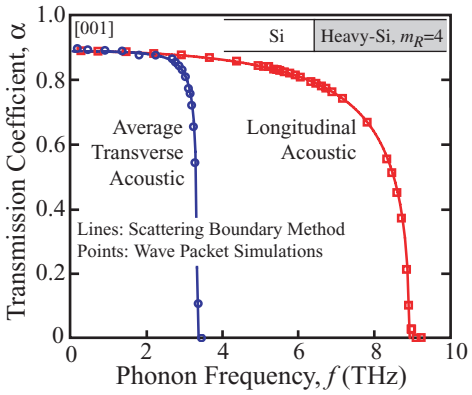

Figure 3: [001] transmission coefficients for a SW Si/heavy-Si interface with $m_R = 4$ predicted from wave-packet MD simulations[46] (points) and the scattering boundary method using lattice dynamics calculations (lines). The scattering boundary method calculations are three orders of magnitude faster than the wave packet simulations.

of the group velocity normal to the interface. The first (second) integral is over the Brillouin zone of the left (right) lead, and the first (second) summation is over phonons moving in the positive (negative) z-direction. The mode-dependent phonon transmission coefficient, α_{LR}, is defined as the fraction of the incident phonon energy that is transmitted from the left lead to the right lead (similar for α_{RL}). The variables f_L and f_R are the mode-dependent phonon distributions in the left and right leads at the lead/junction boundaries. These distributions can be written as

$$f_L(\boldsymbol{\kappa},\nu) = f^{\mathrm{BE}}[\omega(\boldsymbol{\kappa},\nu),T_L] + f'_L(\boldsymbol{\kappa},\nu) \text{ and } f_R(\boldsymbol{\kappa},\nu) = f^{\mathrm{BE}}[\omega(\boldsymbol{\kappa},\nu),T_R] + f'_R(\boldsymbol{\kappa},\nu), \tag{3}$$

where f^{BE} is the equilibrium Bose-Einstein distribution and f'_L and f'_R are the deviations from equilibrium.

If f_L and f_R are assumed to follow f^{BE} at T_L and T_R (i.e., $f'_L = f'_R = 0$), the thermal boundary resistance can be written as[28,39,40]

$$R_E = \left[\frac{1}{8\pi^3}\int_L \sum_{\nu}^{+} \hbar\omega v_z \alpha_{LR} \frac{df^{\mathrm{BE}}}{dT} d\boldsymbol{\kappa}\right]^{-1}, \tag{4}$$

The subscript E denotes that the phonons in the leads follow the equilibrium distribution function. Due to its simplicity, Eq. (4), which is analogous to the Landauer expression for electrical conductance, is the most commonly applied expression for calculating thermal resistance.[38,40,42,50,94–97] It is well known, however, that this expression is inaccurate when the average phonon transmission coefficient approaches unity.[28,98] For example, in a perfect crystal (i.e., a system containing no interface), $\alpha_{LR} = 1$ for all phonon modes, and the incorrect result of a non-zero thermal resistance is predicted. This error results from the assumption that $f'_L = f'_R = 0$.[98]

Evaluation of Eqs. (4) requires specification of the phonon properties. The frequencies and velocities can be obtained from a standard harmonic lattice dynamics calculation.[60,99] Under the assumption of specular and elastic scattering at the interface (i.e., the incident, reflected, and transmitted phonons all have the same frequency), the transmission coefficients can also be predicted from harmonic lattice dynamics calculations.[38,40–43] Of particular note is the scattering boundary method,[41–43] where the atomic detail at the interface is explicitly considered. In this approach, as shown in Fig. 2(b), the system is divided into three parts: the junction region, where atomistic de-

tail is retained, and two semi-infinite crystalline leads, where the vibrational modes (the phonons) are plane waves.† For each phonon incident on the boundary, a harmonic lattice dynamics calculation is performed to determine the wave vectors of the reflected and transmitted phonons (which will have the same frequencies due to the assumption of elastic scattering). Equations of motion for the atoms in the junction are then derived and used to obtain a system of equations that can be solved for the transmission coefficients. *Using lattice dynamics to predict phonon properties naturally includes quantum effects, which are not accessible in classical MD simulations.*

Schelling and co-workers describe a MD approach for predicting transmission coefficients based on monitoring the interaction of a phonon wave-packet with an interface.[46,48,50,63,94,100] The simulations are computationally intensive (an individual run is needed for every phonon mode) and are performed with no thermal background. In Fig. 3, the [001] transmission coefficients for an interface of SW silicon and a species with four times the mass of SW silicon (i.e., "heavy-Si") predicted by my research group using the scattering boundary method are compared to the wave-packet results of Schelling et al.[46] The agreement is excellent, and notably, the scattering boundary method calculations are *three orders of magnitude* faster than the wave-packet simulations.

If the fluctuations are retained, the thermal boundary resistance can be written as[44,98,101]

$$R_{NE} = \left[1 - \frac{1}{8\pi^3}\int_L \sum_\nu^+ \beta_L \alpha_{LR} d\boldsymbol{\kappa} - \frac{1}{8\pi^3}\int_R \sum_\nu^- \beta_R \alpha_{RL} d\boldsymbol{\kappa}\right] R_E, \tag{5}$$

where β is the fraction of the total heat flux carried by each phonon mode in the lead, given by $\beta = \hbar\omega v_z f'/q$. The subscript NE denotes that the phonons in the leads follow a non-equilibrium distribution function. Equation (5) predicts the correct result of zero resistance when no interface is present. Specifying the deviations from the equilibrium distribution is a challenging endeavor, and as such, this formulation has not been widely-applied.[44,50,98,101] One suggested approach is to solve the BTE under the assumption of bulk-like scattering,[44,95] leading to $\beta = (\hbar\omega v_z^2 \tau/k)(\partial f^{\mathrm{BE}}/\partial T)$, where the bulk phonon relaxation times, τ, and thermal conductivity, k, can be found using anharmonic lattice dynamics calculations.[77,78]

To my knowledge, only two comparisons have been made between Eqs. (1), (4), and (5). First, Aubry et al. predicted the thermal boundary resistance of the Σ3(111) and Σ29(001) grain boundaries in SW silicon.[50] The transmission coefficients were obtained from wave-packet simulations. Second, my research group studied a series of epitaxial interfaces of materials modeled using the SW potential and transmission coefficients obtained from the scattering boundary method.[44] In Section 3.1.1, I will discuss my group's results, which are consistent with the findings of Aubry et al., who considered a smaller number of interfaces and only one temperature.

3 Research Program

3.1 Task 1: Resolving Differences Between Thermal Boundary Resistance Predictions

3.1.1 Comparing MD and Phonon-based Predictions

Thermal boundary resistance can be directly predicted using Eq. (1) and MD simulation or by evaluating Eqs. (4) or (5) with phonon properties obtained from lattice dynamics calculations. In this section, I will compare these approaches for two types of interface modeled using the SW potential: (i) a symmetrically-strained Si/Ge interface, and (ii) a series of interfaces between Si and heavy-Si, which differs from Si only in mass by a ratio of m_R. For the Si/heavy-Si interfaces,

†I will study interfaces between crystals. Alloys and amorphous materials are significantly more challenging to model because their normal modes cannot be described by plane waves. Studying interfaces where one side is disordered is beyond the scope of the proposed work, but is a long-term objective.

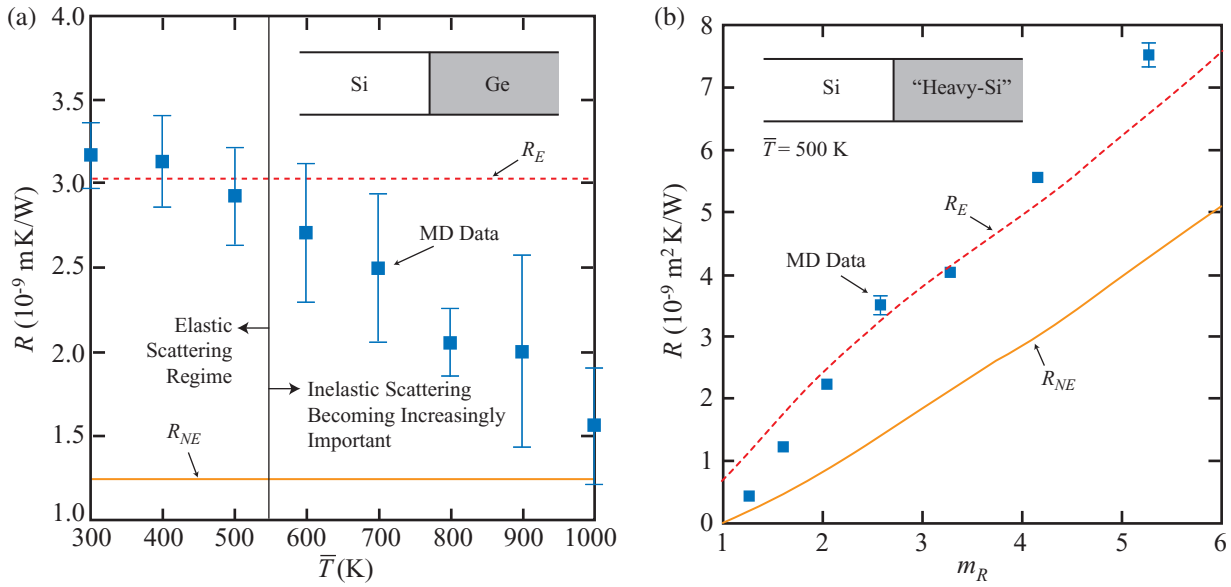

Figure 4: (a) Temperature-dependence of the thermal boundary resistance of a symmetrically-strained Si/Ge interface. (b) Thermal boundary resistance of the Si/heavy-Si interface plotted as a function of mass ratio (m_R) at a temperature of 500 K. The error bars provided for the MD-predicted values represent the 95% confidence interval based on five independent simulations.[44]

mass ratios between 1 and 6 are considered (the Ge/Si mass ratio is 2.6). Each interface is oriented along the (001) crystallographic plane. Because the interfaces contain no defects or roughness that would promote diffuse scattering, I expect that the assumption of specular scattering required for the scattering boundary method calculations is valid.

The MD thermal boundary resistance predictions for the Si/Ge interface between temperatures of 300 K and 1000 K are shown in Fig. 4(a). There is a low-temperature regime below ~500 K where the thermal boundary resistance is temperature-independent and a high-temperature regime in which it decreases with increasing temperature. A temperature-independent thermal boundary resistance in a classical system indicates that the phonon scattering at the interface is elastic. I attribute the temperature-dependence at high temperatures to inelastic phonon interface scattering, which (i) increases with increasing temperature due to increasing anharmonicity of the atomic interactions, and (ii) increases the available channels for conduction.[28] Similar trends of decreasing thermal boundary resistance with increasing temperature have been predicted from MD simulation[55,102] and observed experimentally.[32,33,103]

The MD-predicted thermal boundary resistances for the Si/heavy-Si interfaces at 500 K are shown in Fig. 4(b). Based on the Si/Ge results shown in Fig. 4(a), I expect that the phonons scatter elastically at all the Si/heavy-Si interfaces at this temperature. The thermal boundary resistance decreases monotonically with decreasing mass ratio and approaches zero for $m_R = 1$, the case where no interface is present in the system.

The accuracy of the theoretical expressions for the thermal boundary resistance [Eqs. (4) and (5)] is assessed by comparing their predictions to the MD-predicted values [see Figs. 4(a) and 4(b)]. For the Si/Ge interface, R_E is 3.0×10^{-9} m^2-K/W in the classical limit. This value is in good agreement with the MD prediction of 3.1×10^{-9} m^2-K/W in the elastic scattering regime. For the Si/heavy-Si interfaces, R_E agrees with the MD-predicted values to within 12% for $m_R \geq 2$. As expected, R_E is erroneously non-zero when no interface is present in the system due to the assumption of equilibrium phonon distributions. For the Si/heavy-Si interfaces, R_{NE} decreases

with decreasing mass ratio and is equal to zero when no interface is present in the system, consistent with the MD-predicted trend. For the Si/Ge and Si/heavy-Si interfaces, R_{NE} is 40-60% less than the MD-predicted values in the elastic scattering regime. I attribute the inaccuracy to the assumption of bulk-like non-equilibrium phonon distributions near the interface.

Based on these results, a model that can correctly predict the thermal boundary resistance of an arbitrary interface at any temperature should include inelastic scattering and non-equilibrium phonon distributions. Recent theoretical work suggests that the effects of inelastic scattering can be probed using a Green's function approach.[43,104,105] This technique, however, is theoretically complex and computationally demanding, and has thus far only been applied to molecules. Inelastic scattering has been experimentally observed to become important above the smaller of the Debye temperatures of the materials at an interface.[32] As the Debye temperature of semiconductors and many metals are well above room temperature, I will focus the effort of the proposed work on the specification of the non-equilibrium phonon distributions.

3.1.2 Proposed Work: Predicting Non-equilibrium Phonon Distributions

I propose to determine the non-equilibrium phonon distributions by solving the BTE for the phonon modes on each side of SW Si/Ge and Si/heavy-Si interfaces. The two sides will be coupled through the transmission coefficients predicted using the scattering boundary method. The linearized BTE for phonon mode λ in a system with only a z-direction temperature gradient is

$$v_{z,\lambda}\frac{dT}{dz}\frac{\partial f_\lambda^{\mathrm{B}E}}{\partial T} = \left(\frac{\partial f_\lambda}{\partial t}\right)_{collision}. \tag{6}$$

The steady-state phonon distribution, f_λ, at position $\mathbf{r}$ is such that the rate that phonons enter/leave the neighborhood of $\mathbf{r}$ due to diffusion [left side of Eq. (6)] is balanced by phonon creation and annihilation [right side of Eq. (6), the collision term].[106,107] In a bulk crystal with no defects, the phonon creation and annihilation rates are determined by inelastic multi-phonon scattering processes. Near an interface, however, the phonon creation and annihilation rates will be affected by reflection and transmission at the interface. These effects will lead to non-equilibrium distributions that are different from those calculated assuming only bulk scattering [see the R_{NE} results in Figs. 4(a) and 4(b)]. The collision term in a bulk material can sometimes be modeled using the relaxation time approximation.[74,77,106,107] It is not clear if this approximation is justified for interface systems and I will therefore solve a more general form of the BTE.

I propose to model the collision term as

$$\begin{aligned} k_{\mathrm{B}}T\left(\frac{\partial f_\lambda}{\partial t}\right)_{collision} = \sum_{\lambda'\lambda''}\left[W^I_{\lambda\lambda'\lambda''}(\Psi_{\lambda''}-\Psi_{\lambda'}-\Psi_\lambda)+\frac{1}{2}W^{II}_{\lambda\lambda'\lambda''}(\Psi_{\lambda''}+\Psi_{\lambda'}-\Psi_\lambda)\right] \\ +\sum_{\lambda'}W^{Reflect}_{\lambda\lambda'}(\Psi_{\lambda'}-\Psi_\lambda)+\sum_{\lambda^*}W^{Transmit}_{\lambda\lambda^*}(\Psi_{\lambda^*}-\Psi_\lambda). \end{aligned} \tag{7}$$

Here, $\Psi_\lambda \equiv -f'_\lambda/(\partial f_\lambda^{\mathrm{BE}}/\partial\omega_\lambda)$ and accounts for the deviation of the phonon distributions from equilibrium.[108] The BTEs for all the phonon modes are coupled through the distribution functions and the scattering rates (the W terms, which are not affected by deviations from equilibrium). The first set of summations on the right side of Eq. (7) are over the phonons on the same side of the interface as mode λ and describe type I and II three-phonon interactions. Expressions for the scattering rates $W^I_{\lambda\lambda'\lambda''}$ and $W^I_{\lambda\lambda'\lambda''}$ are available.[77,108–110]

The second(third) summation on the right side of Eq. (7) accounts for changes in the phonon distributions due to two-phonon (i.e., elastic) reflection(transmission) events at the interface. The superscript $*$ denotes phonon modes on the other side of the interface as mode λ. The first step in Task 1 will be to derive expressions for the interface scattering rates, which are not currently

available. I will follow the general procedure outlined by Srivastava for three-phonon, phonon-boundary, and phonon-defect scattering.[107] Based on the forms of these scattering rates, I believe that the interface scattering rates will take the form

$$\begin{aligned} W_{\lambda\lambda'}^{Reflect} &= g_R(f_\lambda^{\mathrm{BE}}, f_{\lambda'}^{\mathrm{BE}}, v_{z,\lambda}, v_{z,\lambda'}, \omega) \times \text{scattering matrix element} \times \text{selection rules criteria} \\ W_{\lambda\lambda^*}^{Transmit} &= g_T(f_\lambda^{\mathrm{BE}}, f_{\lambda^*}^{\mathrm{BE}}, v_{z,\lambda}, v_{z,\lambda^*}, \omega) \times \text{scattering matrix element} \times \text{selection rules criteria.} \end{aligned}$$

The functions g_R and g_T will contain the equilibrium phonon populations and the phonon velocities normal to the interface (both needed to compute the rate at which phonons arrive and leave) and the frequency of the two phonons (which will be the same for elastic scattering). I believe that the scattering matrix element will contain the transmission coefficients found using the scattering boundary method. The selection criteria are imposed in the scattering boundary method, so that the interactions to be included in the summations will be known *a priori* to solving the BTE.

Once expressions for $W_{\lambda\lambda'}^{Reflect}$ and $W_{\lambda\lambda^*}^{Transmit}$ are derived, I will solve the coupled BTEs for the phonon modes on both sides of the interface using a modified version of the iterative procedure developed by Omini and Sparavigna for predicting bulk thermal conductivity.[108,111,112] The bulk procedure is initiated by applying a small temperature gradient to the system and assuming a zeroth-order BTE solution. The coupled BTEs are solved, giving non-equilibrium distributions, and the procedure is repeated until the distributions do not change between iterations. The converged non-equilibrium distributions are then used to calculate the heat flux, which is used in the Fourier law with the applied temperature gradient to obtain the thermal conductivity.

The bulk procedure will be modified to account for the interface. The two sides will be held at temperatures T_L and T_R, which set the temperature difference and are used to evaluate f_λ^{BE}. The two materials may have different thermal conductivities, which will differ from bulk values close to the interface. The applied temperature gradients thus need to be chosen so that the heat flux through the two sides is the same [i.e., $q = (kdT/dz)_L = (T_L - T_R)/R = (kdT/dz)_R$]. I will fix the temperature gradients by taking the bulk thermal conductivities as a first approximation and guessing a heat flux based on the R_E solution. The iterative procedure described in the previous paragraph will then be performed. The resulting non-equilibrium distributions will be used to calculate a heat flux, which will differ from the assumed value. This higher-level iterative procedure (each iteration will contain a complete set of iterations to get the deviations) will continue until the heat flux converges. The converged value will give both the thermal boundary resistance and the modified thermal conductivities at the interface.

Checks will be performed to validate the implementation of the iterative procedure and the derived expressions for the interface scattering rates. First, the calculated heat flux should be the same on both sides of the interface. Second, the calculated heat flux should match that found using Eq. (2). Different values of the applied temperature difference will be tested to ensure that the system is in a linear response regime. When used in Eq. (5), the solved distributions should maintain the good agreement found using Eq. (4) for the Si/Ge and Si/heavy-Si interfaces with $m_R \geq 2$ and predict the correct result for the Si/heavy-Si interfaces as m_R approaches unity.

3.2 Task 2: First Principles Prediction of Thermal Boundary Resistance

3.2.1 From Interatomic Potentials to DFT Calculations

The inputs to a harmonic lattice dynamics calculation are the second-order derivatives of the system potential energy with respect to the equilibrium atomic positions (i.e., the harmonic force constants). An advantageous feature of using lattice dynamics calculations to predict phonon properties is that the force constants only need to be evaluated once for a given atomic structure. Force constants are typically obtained from an interatomic potential, either analytically or

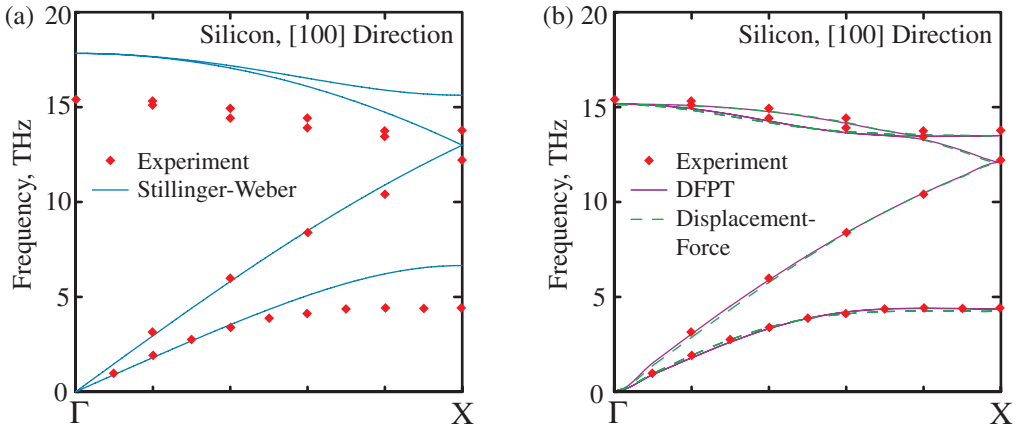

Figure 5: Silicon [100] phonon dispersion curves from (a) experiment[113] and the SW potential, and (b) experiment, density functional perturbation theory (DFPT), and the displacement-force method in DFT.

numerically. Interatomic potentials are usually created by fitting a suitable algebraic expression to experimental data (e.g., lattice constants, elastic constants, defect energies) or predictions from electronic structure calculations (e.g., a potential energy surface). Interatomic potentials are rarely fit to phonon and/or thermal properties.

The [100] silicon dispersion curves predicted by the SW potential are shown in Fig. 5(a) along with experimental data.[113] The SW potential does not reproduce many features of the experimental curves. Notably, the frequencies of the transverse acoustic branch near the X-point are too high, which will lead to an over-prediction of the phonon group velocities, needed in Eqs. (4) and (5). Comparable differences exist in the [110] and [111] directions and for other silicon interatomic potentials.[114] Based on this result alone, we should not expect that the SW potential will predict the experimental thermal conductivity of silicon, which it does not (62 W/m-K at a temperature of 1000 K from MD simulation[115] compared to the experimental value of 31 W/m-K[116]). Inaccuracies will also exist for the thermal boundary resistance. Thus, while the SW potential can be used to explore the nature of phonon physics in diamond structures, as I proposed in Task 1, it does not provide a platform for making predictions that can be used to understand experimental data.

The input to a lattice dynamics calculation need not come from interatomic potentials. Advances in electronic structure calculation methods and increases in computational power have demonstrated that the force constants can be obtained directly from quantum mechanics.[117,118] In an electronic structure calculation, the Schrödinger equation is solved in order to predict the energy of a system of atoms.[119,120] Both the ionic and electronic degrees of freedom are considered. Because the ions are much more massive than the electrons, the ionic and electronic degrees of freedom can be decoupled. The calculation then amounts to solving for the electronic wave functions for a given set of ionic positions. In the DFT approach, the many-electron problem is reduced to solving the Kohn-Sham equation for all the one-electron wave functions.[121–123] Established density functionals exist for all elements. This generality contrasts to interatomic potential-based approaches, where potentials are typically only available for widely-studied materials. Although DFT calculations are computationally demanding, the required time can be reduced by using linear-scaling methods on parallel processors, an area of co-PI Yang's expertise.

Atomic force constants can be obtained from DFT using the displacement-force method,[124–126] density functional perturbation theory (DFPT),[117,118] or the frozen phonon method.[117] Harmonic lattice dynamics calculations using DFT input have successfully predicted force constants and dispersion curves for materials such as silicon, germanium, and III-V semiconductor compounds.[126,127]

In Fig. 5(b), dispersion curves for bulk silicon, generated by my research group using DFPT and the displacement-force method, are shown and compared to experimental results.[113] The agreement is excellent, particularly when compared to the SW predictions shown in Fig. 5(a).

Broido et al.[128] recently used DFT and DFPT to obtain the harmonic and cubic force constants needed to provide the input to an iterative solution to the BTE for predicting thermal conductivity. They found excellent agreement between their predictions for silicon and germanium compared to experimental results (within 5% between temperatures of 100 and 300 K, better agreement than is found with any interatomic potential[108]). This report is one of only a few examples in the literature of a truly first-principles thermal conductivity prediction.[129,130] To my knowledge, force constants from DFT have not been used to predict thermal boundary resistance.

3.2.2 Proposed Work: Thermal Boundary Resistance from First Principles

Despite its tremendous predictive power, the DFT approach has not been embraced by the thermal transport community due to its theoretical and computational complexities. In Task 2, I will demonstrate that DFT calculations can be used to predict the phonon properties needed to evaluate thermal boundary resistance. To develop the methodology, silicon grain boundaries and Si/Ge interfaces will first be considered. Then, I will model a series of semiconductor/metal interfaces for which experimental data is available in order to assess the role of electrons in interfacial thermal transport. The calculations will be performed using Quantum Espresso, a freely-available suite of computer codes based on DFT, plane waves, and pseudo-potentials.[131] The materials to be studied have different lattice constants and the interfaces will be relaxed using an energy minimization procedure I described elsewhere.[44]

I propose to use the displacement-force method to efficiently and accurately obtain the required harmonic force constants. In this approach, the harmonic force constants are calculated directly from their definitions as the second derivatives of the total system energy.[124–126] First, a series of small displacements are applied to selected atoms in a supercell. The resulting forces, which are the first derivatives of the system energy, are calculated via the Hellmann-Feynman theorem. The harmonic force constants are then calculated by numerically differentiating the forces. I prefer the displacement-force method over DFPT due to its transparency in understanding and implementation, particularly for the interface systems to be studied here. Specifically, it has following attributes: (i) Straightforward implementation – DFT calculations are only used to obtain forces. (ii) It is ideally suited for two-level parallelization. The DFT force calculation for each displacement configuration can be highly parallelized and the calculations for different configurations can be performed simultaneously. A linear-scaling DFT approach that can handle up to 10,000 atoms will be used with supercomputing facilities to handle the large supercells required.[85]

Using force constants from bulk DFT calculations, the phonon frequencies and velocities can be obtained from a bulk-phase lattice dynamics calculation. The challenge lies in obtaining the harmonic force constants needed to predict the transmission coefficients using the scattering boundary method. The transmission coefficients for an isolated interface are required, while DFT calculations are inherently periodic. I propose to investigate two approaches for obtaining the required force constants. First, a periodic system containing one interface will be studied. The distance between periodic images of the interface will need to be larger than the range of the atomic interactions. Second, a one-interface structure with hydrogen-terminated ends (to stabilize the surface and prevent reconstruction) and a vacuum gap will be considered. The distance between the interface and the hydrogen atoms will need to be large enough so that the free ends do not affect the behavior at the interface. The size of the vacuum region will be selected to make interactions between the free ends negligible.[132] By using two different computational cells, I will be able to determine which provides the best combination of accuracy and speed.

While the interactions in the SW potential are, by design, limited to the second-nearest neighbors, the interactions in real materials are longer-ranged. To identify the range of the atomic interactions in bulk silicon, I took the output from a Quantum Espresso DFPT calculation and set all the harmonic force constants beyond a certain cutoff radius to zero. I then solved the eigenvalue problem needed to get the phonon frequencies. The results for selected points in the Brillouin zone are shown in Fig. 6. When interactions up to the sixth neighbor shell (0.7 nm) are included, all frequencies are within 1% of their converged values. Based on this result, I will start by studying interfaces 1.5 nm apart for the periodic interface systems and segments 1.5 nm long for the hydrogen-terminated interface systems. As the interface systems may behave differently than a bulk phase, I will also consider larger sizes to ensure system-size independent results.

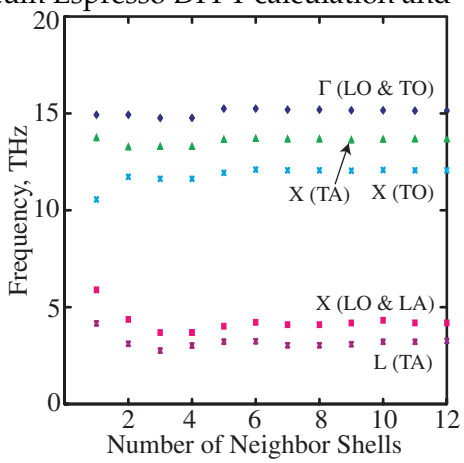

Figure 6: Convergence of DFPT frequencies for bulk Si at selected points in the Brillouin zone. All values are in excellent agreement with experimental data [Fig. 5(b)].

I will first study the The $\Sigma 3(111)$ and $\Sigma 29(001)$ grain boundaries in silicon. Grain boundaries are an important source of phonon scattering in nanostructured silicon, a potential thermoelectric material.[24] As found by Aubry et al.[50] using the SW potential, these two grain boundaries have thermal resistances of 0.1×10^{-9} and 1.3×10^{-9} m^2-K/W, which fall at the low end of the Si/Ge and Si/heavy-Si values [see Fig. 4]. Starting with a single species will simplify the DFT calculations and the low resistances will provide a good test of the theoretical development from Task 1. Modeling grain boundaries, where the crystal orientation is different on either side of the interface, will require modifications to my current implementation of the scattering boundary method. As described by Pettersson and Mahan,[133] larger unit cells and different rules for specifying the wave vectors of the reflected and transmitted must be used, but the procedure is otherwise similar. Si/Ge interfaces will then be modeled. While no experimental measurements exist due to their low thermal resistance, it will be useful to have a theoretical prediction when experimental capabilities improve.

After gaining confidence in the use of DFT calculations to predict thermal boundary resistance, I will model the Cr/Si, Pb/diamond, Au/diamond, and Bi/diamond metal/semiconductor interfaces, for which temperature-dependent experimental measurements are available.[32,39,103] The mechanism by which thermal energy is transmitted across metal/semiconductor interfaces is unknown. The acoustic and diffuse mismatch models ignore the electrons entirely.[28,37] Majumdar and Reddy suggest that the interfacial thermal transport is due to phonon-phonon interactions, with electron-phonon coupling on the metal side of the interface influencing the phonon populations.[134] Huberman and Overhauser,[135] Sargeev,[136] Mahan[29] developed models of varying complexity that directly link the electrons in the metal to the phonons in the semiconductor.

The DFT-based methodology developed in Task 2 presents an opportunity to directly compare a first-principles calculation involving only phonons to experimental measurements. If the results for a particular interface agree, it will be a good indication that electrons do not play an important role. Disagreement will indicate that the electrons do need to be considered, providing a starting point for developing new models to include their effects. The recent work of Mahan[29] is a promising step in this direction. In addition to using experimental data referenced above, I will work closely in this portion of Task 2 with Professor Jonathan Malen (CMU), who has experimental facilities for measuring thermal boundary resistance (see attached letter).

3.3 Task 3: Phonon Transport Near and Across Closely-Spaced Interfaces

3.3.1 Preliminary Results

To this point, the proposed work has focused on isolated interfaces. As discussed in Section 1.1, closely-spaced interfaces exist in materials used in semiconductor and energy conversion devices. The work proposed in Task 3 is motivated by findings made by my research group using MD simulation and lattice dynamics calculations to study SW Si and Ge multi-interface systems:

1. The thermal boundary resistance of an isolated Si/Ge interface is reduced by 25% when 12% species mixing is introduced in the layers immediately adjacent to the interface (i.e., the conductance increases). The same amount of species mixing *reduces* the thermal conductivity of a Si/Ge superlattice with 1.1 nm thick layers by a factor of ten.[62] In multi-interface Si/Ge systems with this same interface separation, the total thermal resistance is within 10% of that predicted using the bulk superlattice thermal conductivity for a 300 nm-long fragment. With species mixing, a fragment with a length of only 90 nm is required.

2. In Fig. 7(a), the thermal resistances predicted by the direct MD method for (i) a Ge thin film bounded by Si leads and (ii) a Si thin film bounded by Ge leads are plotted versus the film thickness. For films thicker than 2 nm, the thermal resistance of the Si thin films is about half of that for the Ge thin films. As I discussed elsewhere,[65] understanding this difference requires using the mode-dependence of the phonon mean free paths to identify if a phonon will travel ballistically or diffusively through the thin film. Further work is required to develop a phonon-based technique that can capture this effect.

3. In Fig. 7(b), MD-predicted thermal resistances of perfect Si/Ge superlattice fragments with layer thicknesses of 1.1 nm and different bounding species (Si&Si, Si&Ge, and Ge&Ge) are plotted versus the number of interfaces in the fragment. The differences in the thermal resistances indicate that phonon transport in multi-layer systems is dependent not only on the composition of the layers, but also on the bounding species.

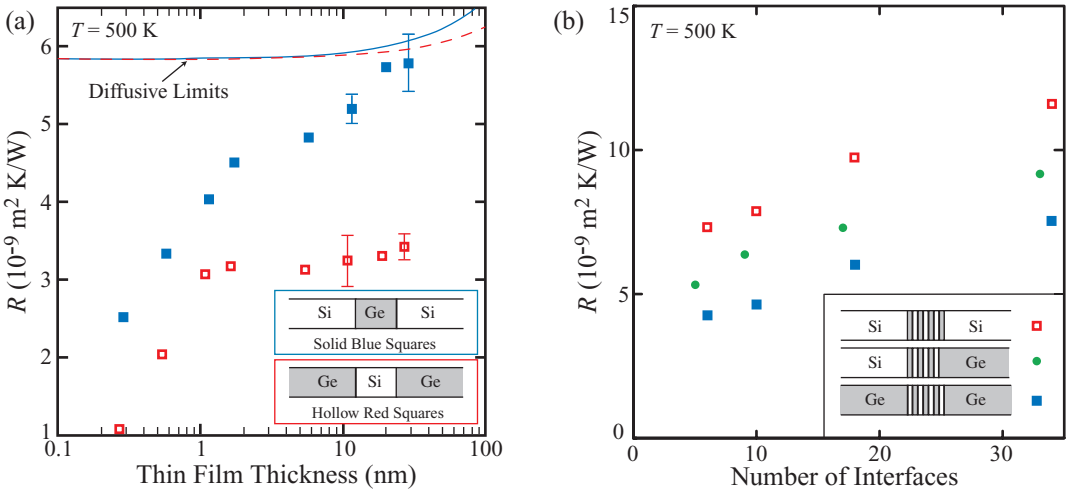

Figure 7: (a) Thermal resistances of SW Si and SW Ge thin films predicted by my research group using MD simulation.[65] The diffusive limits are calculated using the thermal boundary resistance of an isolated interface and the bulk thermal conductivities. The error bars provided for the MD-predicted values represent the 95% confidence interval based on five independent simulations. (b) Effect of bounding species on thermal resistance of Si/Ge superlattice fragments.

3.3.2 Proposed Work

I will use MD simulation and lattice dynamics calculations to probe the effect of species mixing, the formation of Bloch modes, the role of the bounding species, and diffusive/ballistic effects in multi-layer structures. Using these two approaches simultaneously will allow for the identification of when anharmonic (i.e., inelastic) effects emerge, which are only captured in MD simulation.

Interfacial Species Mixing: Species mixing in a superlattice removes the periodicity, which causes phonons to scatter at the interfaces, thus lowering the thermal conductivity.[62] Mixing increases the conductance (i.e. decreases the resistance) of an isolated Si/Ge interface. Based on preliminary data not shown here, a similar effect exists in Si and Ge thin films. I propose to examine how this increased conductance is realized by using the scattering boundary method to predict the mode-dependent transmission coefficients across isolated interfaces and thin films with interfacial species mixing. To do so, unit cells with larger cross-sectional areas than used for the perfect interfaces will need to be studied so as to include an amount of mixing typical of real interfaces. I will take advantage of the resources at the Pittsburgh Supercomputing Center to overcome the additional computational expense.

Transition to Coherent Bloch Modes: The transition in behavior from a single interface to multiple interfaces to a periodic superlattice occurs due to the formation of coherent Bloch modes. The ability to predict when this transition occurs is important in device design. This transition will happen at different points for different phonon modes. To examine the mode-dependent transition, I will use lattice dynamics calculations to determine the local phonon density of states[65,137] along the length of superlattice fragments with and without species mixing. I previously used this technique to determine when bulk dispersive properties emerge in a thin film.[65] By comparing the results to bulk Si, bulk Ge, and Si/Ge superlattice density of states, I will be able to identify how specific modes approach bulk-like characteristics.

Role of Bounding Species: I will use both MD simulation and the scattering boundary method to predict the thermal boundary resistance of single Si/superlattice and Ge/superlattice interfaces. This prediction will allow for the separation of the resistance at the lead/superlattice fragment interfaces from that within the fragment.

My long-term objective is to use the findings from Task 3 to build a phonon-based model for predicting the thermal resistance of multi-interface structures. Input will come from bulk calculations of mean free paths, which will be used to identify the degree to which a mode travels diffusively, and transmission coefficients predicted using the scattering boundary method. Ballistic phonon modes are straightforward to handle, as their transmission coefficients are those predicted by the scattering boundary method. The challenge is the diffusive modes, as phonon-phonon scattering within a multi-interface structure both (i) reduces the transmission coefficient and (ii) create new phonons. Including these effects, particularly (ii), is a significant challenge, and I believe that this work will extend beyond the scope of that proposed here. One potential avenue is to apply the results to parameterize a 1-D model proposed by Simkin and Mahan[138] that captures coherent and incoherent behavior in superlattices.

The work proposed in Task 3 closely matches the interests of Professor Jon Malen (CMU), who uses experimental techniques to examine thermal transport in multi-layer structures for solid state lighting and thermoelectric energy conversion applications (see attached letter). Professor Malen and I will share our results so as to better understand both the theoretical and experimental findings.

4 Broader Impact: Heat Transfer Physics

Engineers must learn and apply new skills as they identify and take on transport problems at the nanoscale. In the realm of thermal transport, knowledge of quantum mechanics, solid state physics, and electromagnetic theory are vital. This emerging field has been called heat transfer physics.[139,140] A successful implementation of heat transfer physics into engineering curricula will include instruction in fundamentals and exposure to state-of-the-art research results.

I taught a graduate course on heat transfer physics in the Spring 2007 semester and will develop a new elective undergraduate course in the proposed work. In these courses, careful effort will be devoted to relating traditional heat transfer analysis to atomic-level behavior. Clear links between the classical heat transfer modes (conduction, convection, and radiation) and the atomistic energy carriers (phonons, electrons, fluid particles, and photons) will be made through discussion of real-world systems (e.g., thermoelectric materials, solar cells, solid state lighting, laser cooling). The conditions under which continuum-level theories become invalid will be carefully presented. Specific examples will include studying experimental results for the thermal conductivity of thin films[141,142] and my group's modeling work on water flow in carbon nanotubes.[143,144] Students will be exposed to fundamental theory (e.g., simple solutions of the Schrodinger equation), simulation tools (e.g., an easy-to-use version of the my group's molecular dynamics research code), and cutting-edge research (e.g., tours of labs on the CMU campus and at the nearby University of Pittsburgh, as well as guest speakers). I will draw on examples from my group's research. For instance, using phonon transport in superlattices to explain the difference between diffusive and ballistic transport and showing how the thermal conductivity of a carbon nanotube is reduced by phonon-fluid particle interactions.

To reach a broader audience, I am currently developing the undergraduate lecture series "Mechanical Engineering from the Nanometer-Up," which I will present in core courses in my department. The lecture developed as part of the proposed work will be on thermoelectric materials and be given in the junior-level heat transfer class that I teach. It will focus on the coupled transport of heat and electricity by phonons and electrons and feature a hand-held thermoelectric device that can heat and cool. Students will work through a simplified design task, where they will optimize both thermal and electrical performance. I am adapting these lectures for high school students under the title "How Small is Small?" As a means to attract a more diverse group of students to science and engineering, I will offer them through existing outreach programs at CMU. These activities include the annual Society for Women Engineers High School Day (in which I have participated since 2005) and the Science and Math Academy at Westinghouse High School, an at-risk Pittsburgh public school.[145]

As heat transfer physics is an emerging area for engineers, it is important to efficiently disseminate new information. I will do this through nanoHUB[70] and thermalHUB,[71] two NSF-supported online resources. My contributions will include: (i) Posting materials related to "Mechanical Engineering from the Nanometer-Up," so that instructors at other universities can develop similar lectures. The posted materials will include presentation slides and audio/visual recordings of the lectures. (ii) Developing an online simulation tool based on the scattering boundary method for demonstrating thermal transport by phonons through a 1-D chain. Users will be able to vary the masses of the atoms and stiffness of the atomic bonds in the lead and junction regions to assess how they influence thermal transport at both the individual phonon- and system-levels.

5 Implementation

The proposed work plan is shown in Fig. 8. The research will be performed by one graduate student who I will advise and guide. One undergraduate student will be hired each summer through CMU programs that bring under-represented minority students from other universities to Pittsburgh for a research experience. The exposure that I will gain through presentations at APS, MRS, and ASME conferences, publications in physics and engineering journals , nanoHUB, thermalHUB, and an annual simulator's meeting that I organize in Pittsburgh[146] will open up new possibilities for collaborations with theorists and experimentalists.

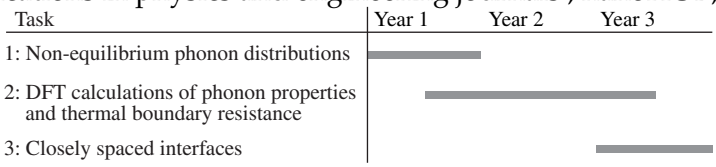

Figure 8: Research task timeline.

6 Summary

The intellectual merit of the proposed work will be found in (i) an improved atomistic foundation for understanding interfacial phonon transport, and (ii) a suite of computational tools for studying phonon transport near and across interfaces at a level of accuracy and detail that is not currently available. With these tools, it will be possible to model thermal transport in any nanostructured material where the transport is dominated by phonons, opening up the possibility of designing materials with tailored thermal transport properties. Specifically, I will:

- Resolve the discrepancies between different thermal boundary resistance models by deriving the phonon-interface scattering rate and then predicting the non-equilibrium phonon distributions that exist at interfaces.
- Demonstrate that DFT calculations can be used to provide the input for lattice-dynamics based thermal boundary resistance models. Use the DFT predictions to assess the role of electrons in thermal transport across metal-semiconductor interfaces.
- Identify how Bloch phonon modes develop as you move from an isolated interface to multiple interfaces to a periodic superlattice and the associated role of interfacial species mixing.

The application of electronic structure calculations for predicting thermal transport properties is exciting. Few researchers are currently exploring this approach, in large part because of the theoretical and computational complexity. My extensive experience in working with atomistic computational tools places me in a unique position to take on this challenging and important research opportunity. Potential future projects include: (i) Extending the first-principles modeling to include polar interfaces (e.g., those involving III-V compounds, where the atomic interactions are longer range), inelastic scattering, electron-phonon interactions, and disordered materials. (ii) Studying thermal transport across interfaces between bulk materials and low-dimensional solids (e.g., nanotubes and nanowires).

The proposed work will broadly impact the wealth of technologically important systems that contain multi-layer components through the general applicability of the analysis tools developed. Proper consideration of the phonon and thermal transport in these systems is critical for the design of high-performance devices. The proposed work will also introduce a broad community (high school, undergraduate, and graduate students) to the field of heat transfer physics though teaching, undergraduate research experience, graduate student training, and community outreach.

7 Results from Previous NSF Support

I am the PI on CBET-0933510 "IDR - Carbon Nanotube Aerogel Networks for Next-Generation Thermal Management," with co-PIs Shelley Anna (CMU), Mohammad Islam (CMU) and Kevin Pipe (University of Michigan), 09/09 – 08/12, $965,874. This project has just begun.

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Alan J. H. McGaughey

Professional Preparation:

McMaster University, Dept. of Mechanical Engineering, Bachelor of Engineering, 1998.
University of Toronto, Dept. of Mechanical and Industrial. Eng, Master of Applied Science, 2000.
University of Michigan, Dept. of Mechanical Engineering, Doctor of Philosophy, 2004.
University of Florida, Dept. of Materials Science and Eng., Postdoctoral Fellow, 2004–2005.

Appointments:

Assistant Professor, Carnegie Mellon University, Dept. of Mechanical Engineering, 2005-
Struminger Junior Faculty Fellow, 2009

Selected Relevant Publications:

1. E. S. Landry and A. J. H. McGaughey, "Thermal boundary resistance predictions from molecular dynamics simulations and theoretical calculations." *Physical Review B* **80**, 165304 (2009).
2. J. E. Turney, E. S. Landry, A. J. H. McGaughey, and C. H. Amon, "Predicting phonon properties and thermal conductivity from anharmonic lattice dynamics calculations and molecular dynamics simulations." *Physical Review B* **79**, 064301 (2009).
3. E. S. Landry and A. J. H. McGaughey, "Effect of interfacial species mixing on phonon transport in semiconductor superlattices." *Physical Review B* **79**, 075316 (2009).
4. A. J. H. McGaughey and M. Kaviany, ``Observation and description of phonon interactions in molecular dynamics simulations." *Physical Review B* **71**, 184305 (2005).
5. A. J. H. McGaughey and M. Kaviany, `` Quantitative validation of the Boltzmann transport equation phonon thermal conductivity model under the single-mode relaxation time approximation." *Physical Review B* **69**, 094303 (2004).

Selected Additional Publications

1. M. Lee and A. J. H. McGaughey, "Energetics of oxygen embedment into unreconstructed and reconstructed Cu(100) surfaces: Density functional theory calculations." To appear in *Surface Science*.
2. J. A. Thomas and A. J. H. McGaughey, "Water flow in carbon nanotubes: Transition to subcontinuum flow." *Physical Review Letters* **102**, 184502 (2009).
3. J. A. Thomas and A. J. H. McGaughey, "Reassessing fast water transport through carbon nanotubes," *Nano Letters* **8,** 2788-2793 (2008).
4. E. S. Landry, M. I. Hussein, and A. J. H. McGaughey, "Complex superlattice unit cell designs for reduced thermal conductivity." *Physical Review B* **77**, 184302 (2008).
5. A. J. H. McGaughey, M. I. Hussein, E. S. Landry, M. Kaviany, and G. Hulbert, `` Phonon band structure and thermal transport correlation in a layered diatomic crystal," *Physical Review B* **74**, 104304 (2006).

Synergistic Activities:

- Developed and taught "Molecular Simulation of Materials," a graduate course offered in the Spring 2006, Spring 2007, and Spring 2010 semesters.
- Developed and taught "Grand Challenges for Engineering (for non-Scientific People)," CMU Osher School of Lifelong Learning, Spring 2009.
- Host of annual Multidisciplinary Simulator's Meeting at CMU.
- Topic Organizer, 2008 and 2009 Summer Heat Transfer Conferences.
- Symposium Organizer, 2009 MS&T Conference and Exhibition.
- Workshop Organizer, Telluride Science Research Center, June 2010.
- Building NTPWiki (http://ntpl.me.cmu.edu/ntpwiki/), an online teaching tool and research resource about nanoscale transport and molecular simulation.
- Developed undergraduate lecture series "Mechanical Eng. from the Nanometer-Up"
- Advised thirteen undergraduate students. Four funded by the CMU Undergraduate Research Initiative. Four completed/ongoing Senior Honors Thesis Projects.
- Member, American Society of Mechanical Engineering, American Physical Society, American Society for Engineering Education, Materials Research Society.
- Reviewer for Physical Review Letters, Reviews of Modern Physics, Journal of Applied Physics, Physical Review B, Applied Physics Letters, Int. Journal of Heat and Mass Transfer, Microscale and Nanoscale Thermophysical Eng., Journal of Heat Transfer, Physics of Fluids, Journal of Physical Chemistry. Proposal reviewer for NSF and DOE.
- Society of Women Engineers High School Day, Fall 2005-2009.
- TechGyrls Coach (a YWCA program that teaches middle-school girls from under-represented Pittsburgh communities about math and science).

Collaborators & Other Affiliations

(i) Collaborators and Co-Editors.

Amon, Cristina (University of Toronto); Anna, Shelley (Carnegie Mellon University); Bain, James (Carnegie Mellon University); Davis, Robert (Carnegie Mellon University); Chung, Jae-Dong (Sejong National University); Hulbert, Greg (University of Michigan); Hussein, Mahmoud (University of Colorado, Boulder); Islam, Mohammad (Carnegie Mellon University); Jordan, Ken (University of Pittsburgh); Li, Ju (University of Pennsylvania); Kaviany, Massoud (University of Michigan); Keblinski, Pawel (Rensellaer Polytechnic Institute); Phillpot, Simon (University of Florida); Pipe, Kevin (University of Michigan); Sinnott, Susan (University of Florida); Sholl, David (Georgia Institute of Technology); Wang, Yang (Pittsburgh Supercomputing Center); Yang, Judy (University of Pittsburgh).

(ii) Graduate and Postdoctoral Advisors.

Charles Ward, University of Toronto (M. A. Sc), Massoud Kaviany, University of Michigan (Ph.D.) Simon Phillpot, Susan Sinnott, University of Florida, Judith Yang, University of Pittsburgh (Postdoctoral).

(iii) *Thesis Advisor and Postgraduate Scholar Sponsor* (Total: 5 Ph.D. and 1 M.S. students):

Eric Landry (M.S, 2007, Ph.D, 2009), Joe Turney (Ph.D., 2009, co-advised with Cristina Amon), John Thomas (Ph.D, expected 2010), Minyoung Lee (Ph.D., expected 2010), Jason Larkin (Ph.D., expected 2013).

Yang Wang

Pittsburgh Supercomputing Center
300 South Craig Street
Carnegie Mellon University
Pittsburgh, PA 15213
E-mail: ywg@psc.edu

Professional Preparation

Ph.D.	Physics, Florida Atlantic University, Boca Raton, FL., 1993 Department of Physics, Florida Atlantic University
M.E.	Electrical Engineering, Chinese Academy of Sciences, Beijing, China, 1985
B.S.	Physics, University of Science and Technology of China, Hefei, China, 1982

Appointments

1996-present	Senior Computational Scientist, Pittsburgh Supercomputing Center, Carnegie Mellon University, Pittsburgh, PA
1993-1996	Postdoctoral Researcher, Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, TN

Awards and Honors

1998	*Gorden-Bell prize* for best achievement in high-performance computing
2000	Year 2000 *Permanent Research Collection on Information Technology at the Smithsonian's National Museum of American History*

Graduate and Post-doctoral Advisors

Dr. J. S. Faulkner	Dr. G. M. Stocks
Department of Physics	Metals and Ceramics Division
Florida Atlantic University	Oak Ridge National Laboratory
Boca Raton, FL 33431	Oak Ridge, TN 37831
1-561-297-3429	1-865-574-5163

Five Publications Closely Related to the Proposed Project

1 Yang Wang, Stocks G.M., Rusanu A., Nicholson D.M.C., Eisenbach M., Qiming Zhang, Liu J.P., "Electronic and Magnetic Structure of $L1_0$-FePt Nanoparticle Embedded in FePt Random Alloy," *IEEE Transactions on Magnetics,* 43 (6), 3103-3105 (2007).

2 Ezio Bruno, Leon Zingales, and Yang Wang, "Charge distributions in metallic alloys: A charge-excess functional theory approach", Phys. Rev. Lett., **91**, 166401 (2003)

3 Yang Wang, G.M. Stocks, D.M.C. Nicholson, W.A.Shelton, V.P. Antropov and B.N. Harmon, "Non-collinear Magnetic Structure in $Ni_{0.35}Fe_{0.65}$", J. Appl. Phys., **81**, 3873 (1997)

4 Yang Wang, G.M. Stocks, D.M.C. Nicholson, and W.A. Shelton, "The First Principles O[N] LSMS Method and Its Applications to Magnetic Structure of Alloys", Int. J. Computers & Math. Appl., **35**, 85 (1998)

5 Yang Wang, G.M. Stocks, W.A. Shelton, D.M.C. Nicholson, W.M. Temmerman, and Z. Szotek, "Order-N Multiple Scattering Approach to Electronic Structure Calculations", Phys. Rev. Lett., **75**, 2867 (1995)

Five Other Related Publications

1 Yang Wang, M. Widom, D.M.C. Nicholson, M. Mihalkovic, and S. Naidu, "The electronic and magnetic structure of Fe-based bulk amorphous metals: An ab-initio approach", *Mat. Res. Soc. Symp. Proc.* **754**, 439 (2003)

2 J.S. Faulkner, Yang Wang, and G.M. Stocks, "Core Level Chemical Shifts in Metallic Alloys", Phys. Rev. Lett., **81**, 1905 (1998)

3 J.S. Faulkner, Yang Wang, G.M. Stocks, "Coulomb Energies in Alloys", Phys. Rev. B, **55**, 7492 (1997)

4 J.S. Faulkner, Yang Wang, G.M. Stocks, "An Observation on the Density Functional Theory of Electrons in Extended Systems", Phys. Rev. B **52**, 17106 (1995)

5 Yang Wang, G.M. Stocks, D.M.C. Nicholson, and W.A. Shelton, "Spin-Polarized KKR-CPA Calculations for Ferromagnetic CuNi Alloys", *Alloy Modeling and Design*, TMS proceedings, 81 (1994)

Synergistic Activities

Yang Wang is a staff member of Parallel Applications Group in Pittsburgh Supercomputing Center. His primary responsibility includes high performance software development for scientific applications. His research interests include methodology and algorithm development for computational materials science and computational fluid dynamics, computer simulation techniques and applications, parallel programming for distributed or shared memory computer systems, object oriented software development, and computational finance and economics. He is credited with more than fifty scientific journal publications and serves as a referee for Physical Review B, Physical Review Letter, and Journal of Physics: Condensed Matter. He was a recipient of Gordon-Bell Prize for best achievement in high-performance computing. His work on developing and implementing the LSMS method, the first scientific application software that achieves teraflop performance, has been included in Year 2000 Permanent Research Collection on Information Technology at the Smithsonian's National Museum of American History. He is a member of American Physical Society and Materials Research Society.

Collaborators

- G.M. Stocks, D.M.C. Nicholson, Oak Ridge National Laboratory
- J.S. Faulkner, Florida Atlantic University
- M. Widom, Carnegie Mellon University
- R.Q. Wu, University of California at Irvine
- Noam Bernstein, Naval Research Laboratory

SUMMARY PROPOSAL BUDGET

YEAR 1

FOR NSF USE ONLY		
PROPOSAL NO.	DURATION (months) Proposed	Granted
AWARD NO.		

ORGANIZATION
Carnegie-Mellon University

PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR
Alan McGaughey

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-months CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Alan McGaughey**	0.00	0.00	1.00	$ **9,167**	$
2. **Yang Wang**	1.00	0.00	0.00	**7,173**	
3.					
4.					
5.					
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00	**0**	
7. (**2**) TOTAL SENIOR PERSONNEL (1 - 6)	1.00	0.00	1.00	**16,340**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL SCHOLARS	0.00	0.00	0.00	**0**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.00	0.00	0.00	**0**	
3. (**1**) GRADUATE STUDENTS				**24,150**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**1**) OTHER				**37,485**	
TOTAL SALARIES AND WAGES (A + B)				**77,975**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**3,856**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**81,831**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)				**3,000**	
2. FOREIGN				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **0**					
2. TRAVEL **0**					
3. SUBSISTENCE **0**					
4. OTHER **0**					
TOTAL NUMBER OF PARTICIPANTS (**0**) TOTAL PARTICIPANT COSTS				**0**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**1,000**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**443**	
5. SUBAWARDS				**0**	
6. OTHER				**278**	
TOTAL OTHER DIRECT COSTS				**1,721**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**86,552**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **MTDC (Rate: 55.3500, Base: 49066)**					
TOTAL INDIRECT COSTS (F&A)				**27,158**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**113,710**	
K. RESIDUAL FUNDS				**0**	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ **113,710**	$

M. COST SHARING PROPOSED LEVEL $ **0** AGREED LEVEL IF DIFFERENT $

PI/PD NAME
Alan McGaughey

ORG. REP. NAME*

FOR NSF USE ONLY		
INDIRECT COST RATE VERIFICATION		
Date Checked	Date Of Rate Sheet	Initials - ORG

 ***ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET**

SUMMARY PROPOSAL BUDGET

YEAR 2

FOR NSF USE ONLY		
PROPOSAL NO.	DURATION (months) Proposed	Granted
AWARD NO.		

ORGANIZATION
Carnegie-Mellon University

PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR
Alan McGaughey

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-months CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Alan McGaughey**	0.00	0.00	1.00	$ **9,533**	$
2. **Yang Wang**	1.00	0.00	0.00	**7,424**	
3.					
4.					
5.					
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00	**0**	
7. (**2**) TOTAL SENIOR PERSONNEL (1 - 6)	1.00	0.00	1.00	**16,957**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL SCHOLARS	0.00	0.00	0.00	**0**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.00	0.00	0.00	**0**	
3. (**1**) GRADUATE STUDENTS				**24,750**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**41,707**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**4,002**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**45,709**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)				**3,000**	
2. FOREIGN				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **0**					
2. TRAVEL **0**					
3. SUBSISTENCE **0**					
4. OTHER **0**					
TOTAL NUMBER OF PARTICIPANTS (**0**) TOTAL PARTICIPANT COSTS				**0**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**1,000**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**456**	
5. SUBAWARDS				**0**	
6. OTHER				**39,647**	
TOTAL OTHER DIRECT COSTS				**41,103**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**89,812**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **MTDC (Rate: 55.3500, Base: 50453)**					
TOTAL INDIRECT COSTS (F&A)				**27,926**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**117,738**	
K. RESIDUAL FUNDS				**0**	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ **117,738**	$

M. COST SHARING PROPOSED LEVEL $ **0** AGREED LEVEL IF DIFFERENT $

PI/PD NAME
Alan McGaughey

ORG. REP. NAME*

FOR NSF USE ONLY		
INDIRECT COST RATE VERIFICATION		
Date Checked	Date Of Rate Sheet	Initials - ORG

 ***ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET**

SUMMARY PROPOSAL BUDGET

YEAR 3

FOR NSF USE ONLY		
PROPOSAL NO.	DURATION (months) Proposed	Granted
AWARD NO.		

ORGANIZATION
Carnegie-Mellon University

PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR
Alan McGaughey

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-months CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Alan McGaughey**	0.00	0.00	1.00	$ **9,915**	$
2. **Yang Wang**	1.00	0.00	0.00	**7,684**	
3.					
4.					
5.					
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00	**0**	
7. (**2**) TOTAL SENIOR PERSONNEL (1 - 6)	1.00	0.00	1.00	**17,599**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL SCHOLARS	0.00	0.00	0.00	**0**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.00	0.00	0.00	**0**	
3. (**1**) GRADUATE STUDENTS				**25,350**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**42,949**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**4,153**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**47,102**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)				**3,000**	
2. FOREIGN				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **0**					
2. TRAVEL **0**					
3. SUBSISTENCE **0**					
4. OTHER **0**					
TOTAL NUMBER OF PARTICIPANTS (**0**) TOTAL PARTICIPANT COSTS				**0**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**1,000**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**470**	
5. SUBAWARDS				**0**	
6. OTHER				**41,625**	
TOTAL OTHER DIRECT COSTS				**43,095**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**93,197**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **MTDC (Rate: 55.3500, Base: 51870)**					
TOTAL INDIRECT COSTS (F&A)				**28,710**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**121,907**	
K. RESIDUAL FUNDS				**0**	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ **121,907**	$

M. COST SHARING PROPOSED LEVEL $ **0** AGREED LEVEL IF DIFFERENT $

PI/PD NAME
Alan McGaughey

ORG. REP. NAME*

FOR NSF USE ONLY		
INDIRECT COST RATE VERIFICATION		
Date Checked	Date Of Rate Sheet	Initials - ORG

 ***ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET**

SUMMARY PROPOSAL BUDGET

Cumulative

FOR NSF USE ONLY		
PROPOSAL NO.	DURATION (months) Proposed	Granted
AWARD NO.		

ORGANIZATION: **Carnegie-Mellon University**

PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR: **Alan McGaughey**

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-months CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Alan McGaughey**	0.00	0.00	3.00	$ **28,615**	$
2. **Yang Wang**	3.00	0.00	0.00	**22,281**	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00	**0**	
7. (**2**) TOTAL SENIOR PERSONNEL (1 - 6)	3.00	0.00	3.00	**50,896**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL SCHOLARS	0.00	0.00	0.00	**0**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.00	0.00	0.00	**0**	
3. (**3**) GRADUATE STUDENTS				**74,250**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**1**) OTHER				**37,485**	
TOTAL SALARIES AND WAGES (A + B)				**162,631**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**12,011**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**174,642**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)				**9,000**	
2. FOREIGN				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **0**					
2. TRAVEL **0**					
3. SUBSISTENCE **0**					
4. OTHER **0**					
TOTAL NUMBER OF PARTICIPANTS (**0**) TOTAL PARTICIPANT COSTS				**0**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**3,000**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**1,369**	
5. SUBAWARDS				**0**	
6. OTHER				**81,550**	
TOTAL OTHER DIRECT COSTS				**85,919**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**269,561**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS (F&A)				**83,794**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**353,355**	
K. RESIDUAL FUNDS				**0**	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ **353,355**	$

M. COST SHARING PROPOSED LEVEL $ **0** AGREED LEVEL IF DIFFERENT $

PI/PD NAME: **Alan McGaughey**

ORG. REP. NAME*

FOR NSF USE ONLY		
INDIRECT COST RATE VERIFICATION		
Date Checked	Date Of Rate Sheet	Initials - ORG

C ***ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET**

Budget Justification

Funds are requested to:

- Support one graduate student for the duration of the project (tuition and stipend).
- Provide one month of summer support per year for PI McGaughey.
- Provide one month of calender support for co-PI Wang.
- Allow the PI and the graduate student to attend a domestic conference each year to disseminate research results ($3K/year).
- Computing supplies (replacement hard drives, network cards, etc.) to be used exclusively for award-related activities that are necessary and exclusively needed for the successful completion of the project ($1000/year).
- Computing support at the Pittsburgh Supercomputing Center for Wang to pay into an existing cost pool for supporting desktop computing, printing resources, access to the national internet infrastructure, administrative staff for account administration, usage reporting, and other personnel costs ($443, $456, and $470 in Years 1, 2, and 3) .
- Materials and supplies costs at the Pittsburgh Supercomputing Center for Wang to cover books, printing costs, express mail, memberships/dues, equipment less than $5,000, and software less than $5,000 (calculated as 3.14% of salary and fringe benefits).

Current and Pending Support

Investigator: Alan McGaughey

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Multiscale Atomistic Simulation of Metal-Oxygen Surface Interactions: Methodological Development, Theoretical Investigation and Correlation with Experiment (co-PI, PI: Judith Yang, other co-PIs: Simon Phillpot and Susan Sinnott)

Source of Support: Department of Energy

Total Award Amount: $ 641,301 Total Award Period Covered 10/01/2007-08/31/2010

Location of Project: University of Pittsburgh

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr: 0.5

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Multiscale modeling of phase change materials (PI, co-PI: James Bain)

Source of Support: Pennsylvania Infrastructure Technology Alliance

Total Award Amount: $ 44,175 Total Award Period Covered 01/01/2009-06/30/2010

Location of Project: Carnegie Mellon University

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: IDR - Carbon Nanotube Aerogel Networks for Next-Generation Thermal Management (PI, co-PIs: Shelley Anna, Mohammad Islam, and Kevin Pipe)

Source of Support: National Science Foundation

Total Award Amount: $ 965,874 Total Award Period Covered: 09/01/09-08/31/12

Location of Project: Carnegie Mellon University

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr: 0.5

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Quantum Mechanics Driven Prediction of Nanostructure Thermal Conductivity

Source of Support: Air Force Office of Scientific Research

Total Award Amount: $ 358,846 Total Award Period Covered 01/01/2010-12/31/2012

Location of Project: Carnegie Mellon University

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr: 1.0

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Thermal Conductivity and Interface Thermal Conductance: Quantum Mechanics-Driven Prediction and Development of an Inexpensive and Accessible Measurement Technique (PI, co-PI: Jonathan Malen)

Source of Support: NIST

Total Award Amount: $ 809,440 Total Award Period Covered 09/01/2009-08/31/2012

Location of Project: Carnegie Mellon University

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr: 1.0

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Stirling MicroCooler Array with Elemental In-Plane Flow (co-PI, PI: Gary Fedder, other co-PIs: William Anderson, Matthew Moran, Shi-Chune Yao)

Source of Support: DARPA

Total Award Amount: $ 4,717,822 Total Award Period Covered 01/01/2010-06/30/2014

Location of Project: Carnegie Mellon University

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr: 1.0

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Multiscale Study of Heat Generation, Thermal Resistance, and Enhanced Dissipation by Heat-pipe heat-sinks in Blue and Green LEDs (co-PI, PI: Jonathan Malen, other co-PI: Robert Davis)

Source of Support: DOE

Total Award Amount: $ 1,832,046 Total Award Period Covered 01/01/2010-12/31/2012

Location of Project: Carnegie Mellon University

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr: 1.0

Current and Pending Support

(See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Yang Wang	Other agencies (including NSF) to which this proposal has

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: Teragrid Resource Partners

Source of Support: NSF
Total Award Amount: $52,001,250 Total Award Period Covered: 8/1/2005 – 3/31/11
Location of Project: Carnegie Mellon University and University of Pittsburgh
Person-Months Per Year Committed to the Cal: 7.2 Acad: Sumr:

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: ETF Grid Infrastructure Group: Providing System Management and Integration for the TeraGrid

Source of Support: University of Chicago (NSF)
Total Award Amount: $4,724,417 Total Award Period Covered: 8/1/05 – 7/31/10
Location of Project: Carnegie Mellon University and the University of Pittsburgh
Person-Months Per Year Committed to the Cal: 4.8 Acad: Sumr:

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: Phonon Transport Near and Across Seminductor Interfaces

Source of Support: NSF
Total Award Amount: $ 353,355 Total Award Period Covered: 9/1/11 – 8/31/13
Location of Project: Carnegie Mellon University
Person-Months Per Year Committed to the Cal: 1.0 Acad: Sumr:

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: Energy Frontier Center for Defect Physics in Structural Materials (CDP) {AWARDED)

Source of Support: DOE (through ORNL)
Total Award Amount: $ 100,000 Total Award Period Covered: 10/21/09 – 9/31/14
Location of Project: Carnegie Mellon University
Person-Months Per Year Committed to the Cal: 2.76 Acad: Sumr:

Support: ☒ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Cal: Acad: Sumr:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Facilities, Equipment, and Other Resources for Alan McGaughey

Computer

Seven personal computers, one web server, an 11-node Beowulf Linux cluster, and a 48-node Beowulf Linux cluster. McGaughey and his research group have developed lattice dynamics computer codes suitable for the proposed tasks. They have access to Quantum Espresso and a user license for VASP, both of which are computer codes for performing density functional theory calculations.

McGaughey holds a development grant at the Pittsburgh Supercomputing Centre (no cost).

Office

One faculty office and one graduate student office.

Other

Shared secretarial support (1/5 time).

Major Equipment

Parts of McGaughey's computational work will be carried out on a 48-processor Beowulf Linux cluster installed in September 2006 and expanded in July 2008. The system is housed in Carnegie Mellon Computer Facilities space, with suitable power and cooling capabilities, and uninterrupted power supplies. The system contains one head node and twelve slave nodes which do the computations, and can be accessed from anywhere in the world. The original eight nodes have two AMD Opteron 275 Dual Core Processors (i.e., four processors per node), 2 GB of RAM, and an 80 GB hard drive. The four nodes added in the expansion have two AMD Opteron 2218 Dual Core Processors, 4 GB of RAM, and an 80 GB hard drive. The system runs on the CBeST v3.0 Beowulf cluster software, custom installed on the system for high performance computing.

Facilities, Equipment and Other Resources
at the Pittsburgh Supercomputing Center
Carnegie Mellon University

Computing Resources

PSC's Cray XT3, *bigben*, consists of 2,068 2.6 GHz dual-core AMD Opterons with 2 GB of memory per processor linked by a Cray proprietary high performance interconnect with a link bandwidth of 6.4 GB/s. This machine provides peak aggregate speed greater than 21 Tflop/s with 4 TB of memory. Bigben is best suited to large process count, message-passing applications. An additional twenty-two Service and I/O nodes, also using 2.6 GHz dual-core Opterons, support user logins, file system connections, and access to the TeraGrid Wide Area Network. All compute and service nodes access a high-performance 200 TB disk array for temporary storage as well as connection to PSC's *bessemer* shared, central file system. Both the local and shared storage systems use the Lustre file system architecture.

For applications requiring vast shared memory, high-productivity programming models, and/or moderate parallelism with a high-performance system-wide interconnect, PSC recently installed two SGI Altix 4700 systems. The first, *pople*, offers 768 Intel Itanium 2 dual-core "Montvale" processors with peak aggregate speed of 5.1 Tflop/s and 1.5 TB of shared memory. The second, *salk*, is administered for the National Resource for Biomedical Supercomputing (NRBSC) and offers 144 Montvale processors providing a peak aggregate speed of 0.96 Tflop/s with 288 GB shared memory. These systems support advanced programming languages and models including UPC and Star-P. Both of these systems entered production service on July 1, 2008.

PSC operates several Linux clusters for biomedical and computer science research, as well as several high-end servers and powerful workstations for development, analysis, and visualization tasks. A 40 processor 1.4 GHz Opteron cluster, *codon,* supported by the NRBSC, is dedicated to biomedical application development. The *codon* cluster is currently being upgraded to ~200 2.5 GHz Xeon cores.

The Cray XT3 (bigben) and the larger SGI Altix (pople) are part of the National Science Foundation's TeraGrid, an integrated national system of cyberinfrastructure. These systems are linked to high-end TeraGrid resources by a 30 Gb/s optical network.

Mass Storage

Archival storage for PSC systems is provided by an SGI Altix 450 server running the Data Migration Facility (DMF) software. Two STK storage silos equipped with STK 9940B cartridge tape drives provide ~3 PB of data storage. A system of Cache Nodes (CNs) with high-speed links to PSC supercomputers augments the core archival storage system by providing a large primary disk cache.

Network Facilities

Network facilities at the Pittsburgh Supercomputing Center consist of production and research LAN, MAN, and WAN infrastructures. Network technology used for the LAN infrastructure consists of switched Ethernet ranging in speeds from 10 Mb/s to 10 Gb/s. The MAN infrastructure associated with PSC uses SONET, Ethernet, and DWDM technologies. Its central components are the DWDM network which carries 3 OC-192 links that connect to the Extensible Teragrid Facility (ETF) backplane network via National Lambda Rail and a 10 Gigabit Ethernet connection between the Three Rivers Optical Exchange (3ROX) and the supercomputing facility at the Westinghouse Energy Center.

PSC's WAN connections are provided by 3ROX, a regional network aggregation point that provides high-speed commodity and research network access primarily to sites in Western and Central Pennsylvania and West Virginia. 3ROX is based at Carnegie Mellon University and is operated and managed by the Pittsburgh Supercomputing Center. While the primary focus of 3ROX is to provide cost effective, high capacity, state-of-the-art network connectivity to the university community, this infrastructure also provides well-defined network services to both community (K-12, government) and commercial entities in Western Pennsylvania. University member sites currently include Carnegie Mellon University, the Pennsylvania State University, the Pittsburgh Supercomputing Center, the University of Pittsburgh, Norfolk State University, and West Virginia University. 3ROX's commodity Internet component consists of multiple high performance WAN connections to major Internet service providers, including gigabit Ethernet connections to Sprint and Global Crossing. The research component of 3ROX includes a gigabit Ethernet connection to the Internet2 network. In addition to the Internet2 connection, 3ROX also has a 10 Gigabit Ethernet connection to National Lambda Rail's PacketNet, a nationwide routed IP network that includes a "breakable IP" service. Explicit routing is used to maintain the AUP policies associated with the various production and research network infrastructures

Carnegie Mellon

Mechanical Engineering Department
Carnegie Mellon University
5000 Forbes Avenue
Pittsburgh, Pennsylvania 15213-3890
(412) 268-2500
Fax: (412) 268-3348

October 29, 2009

Dear Alan,

I am very excited about the possibility of collaborating with you on the project "Phonon Transport Near and Across Semiconductor Interfaces." Thermal transport across interfaces is of critical importance in several energy-related technologies that I am currently studying, including light emitting diodes for solid-state lighting and thermoelectric devices for scavenging waste heat.

The primary thrust of my lab's research is experimental characterization of thermal conductance and conductivity in thin films, superlattices, and self assembled monolayers. The interface plays a vital and misunderstood role in the observed thermal conductance of these structures—in particular, the electron-phonon interactions at the interface and coherent phonon effects in superlattice structures. I have developed a technique, Fiber Aligned Thermal Interrogation (FATI), to probe thermal transport in these structures. The prototype FATI setup was capable of measuring thermal conductances on the order of 30 W/m^2-K, but future generations of FATI will be capable of resolving conductances in excess of 100 W/m^2-K, making it comparable to TDTR and 3-omega techniques. I fully expect that your DFT studies will identify metal-semiconductor interfaces and superlattice structures that are within this measurable range.

I currently have a graduate student working on thermal transport in blue/green LEDs, made from GaAs/InGaAs superlattices. Interfaces play a key role in these structures, and we are therefore eager to learn more about the energy transport processes at interfaces by pairing your predictions with our experimental observations. I will not require any additional support from you to collaborate on these studies.

All the best,

Jonathan Malen
Tel: (412) 268-4667
Fax: (412) 268-3348
Email: jonmalen@andrew.cmu.edu