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	5b. GRANT NUMBER
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7. PERFORMING ORGANIZATION NAMES AND ADDRESSES University of Maryland - College Park Office of Research Administration 3112 Lee Building 7809 Regents Drive College Park, MD 20742 -5141	8. PERFORMING ORGANIZATION REPORT NUMBER
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14. ABSTRACT
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a. REPORT UU	b. ABSTRACT UU	c. THIS PAGE UU	19b. TELEPHONE NUMBER 301-405-4543

**RPPR Final Report**  
as of 03-Jan-2019

Agency Code:

Proposal Number: 65404MA

**Agreement Number: W911NF-14-1-0330**

**INVESTIGATOR(S):**

**Name:** Peter Chung  
**Email:** pchung15@umd.edu  
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**Principal:** Y

Organization: **University of Maryland - College Park**

Address: Office of Research Administration, College Park, MD 207425141

Country: USA

DUNS Number: 790934285

EIN: 526002033

**Report Date:** 22-Mar-2015

Date Received: 02-Jan-2019

**Final Report** for Period Beginning 23-Jun-2014 and Ending 22-Dec-2017

**Title:** Techniques for Phonon Superposition Modeling of Shocks and Waves in Solids Research Area 3:

Mathematics - Numerical Analysis

**Begin Performance Period:** 23-Jun-2014

**End Performance Period:** 22-Jun-2018

**Report Term:** 0-Other

Submitted By: Peter Chung

Email: pchung15@umd.edu

Phone: (301) 405-4543

**Distribution Statement:** 1-Approved for public release; distribution is unlimited.

**STEM Degrees:** 3

**STEM Participants:** 6

**Major Goals:** A new approach for modeling phonons will be developed and the modeling errors will be estimated and determined numerically. The approach targets the study of non-equilibrium processes and is based on fundamental principles of quantum field theory as applied to phonons. The new computational methods will be developed and their solutions compared to solutions from an equilibrium-based approach which is representative of methods based on the Boltzmann Transport Equation. The possible advance enabled by capability of studying non-equilibrium phonons is the modeling of mechanical processes such as shock loading at mesoscopic length scales built-up from nanoscopic information.

1. Develop a novel computational method for modeling phonons
2. Perform analysis of computational and numerical errors.
3. Investigate phonons in Army-relevant materials.
4. Develop novel computational method for studying phonons in materials with defects
5. Develop capabilities for the modeling of phonon devices.

**Accomplishments:** 1. Develop a novel computational method for modeling phonons

We developed a new full-Brillouin zone method that successfully predicted anisotropic effects in ballistic AND diffusive carriers. The method could account for Brillouin zone anisotropy as well as anisotropy due to so-called Born von Karman boundary conditions. The results were published in "Computer Methods in Applied Mechanics and Engineering". Another article is currently planned that examines the physics implications in real materials through a more careful examination of the anisotropy predictions and validation.

A review article was published in the "Journal of Materials Science". The article describes many of the computational techniques presently available along with extensive discussions of the benefits and limitations that are important for future developments.

2. Perform analysis of computational and numerical errors.

In the study of the novel computational method for objective 1, we examined the mathematical convergence properties of the algorithm as well as the error estimates for solutions to the phonon Boltzmann Transport Equation. These results were also published in the article in "Computer Methods in Applied Mechanics and Engineering".

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### 3. Investigate phonons in Army-relevant materials.

Phonon mechanisms were studied in the material molybdenum disulfide in collaboration with ARL scientists Dr. Madan Dubey and Dr. Raju Namburu. A journal paper was published in "Nano Research".

Collaborative research was performed with ARL scientist Dr. Sina Najmaei on a material of significant Army interest in Hafnium Disulphide. Numerous joint conference papers have now been submitted and accepted. Several journal articles are planned for the near future (in 2019).

We also investigated phonons in the energetic material RDX. It has led to the first phonon-based cook-off study of an energetic. A refereed conference paper was accepted for publication.

### 4. Develop novel computational method for studying phonons in materials with defects

In the last year of the project, we have continued the examination of phonon modeling for defects using neural network modeling approaches. This research has been presented at the World Congress in Computational Mechanics this year. An archival publication is pending.

### 5. Develop capabilities for the modeling of phonon devices.

A novel design for a phonon filtering device was developed using the code written during this project. The work was published in the International Journal of Heat and Mass Transfer and has drawn interest from ARL to fabricate and experimentally examine the design ideas. A CRADA is in preparation to work collaboratively with the ARL research team developing the experiments.

**Training Opportunities:** Mr. Efrem Perry and Mr. Mark Butrico were supported during the school year as paid undergraduate interns during 2018. Mr. Mark Butrico went on to intern for ARL during the summer of 2018 and contributed to an journal paper in Scientific Reports.

**Results Dissemination:** In the final year of the research:

1. Undergraduate intern sponsorship of Efrem Perry and Mark Butrico during the spring semester of 2018.
2. Published 1 journal article in International Journal of Heat and Mass Transfer.
3. Biweekly teleconference collaborations with Army Research Laboratory Scientists
  - a. 1 journal article with ARL co-authors in progress.
  - b. CRADA in progress (likely to officially start in 2019)
  - c. 2 joint conference papers submitted and accepted to appear in 2019.
4. 1 refereed conference paper to International Detonation Symposium presented and published.
5. 1 invited lecture at TMS2018 in Phoenix.
6. 2 talks delivered at WCCM 2018 in New York, NY in July 2018
7. 2 talks submitted and accepted to appear at MRS Spring Symposium and APS March Meeting both in 2019.

**Honors and Awards:** 1. Invited lecture at 2018 TMS Meeting in Phoenix, AZ in June 2018.

### Protocol Activity Status:

**Technology Transfer:** Extensive biweekly interactions have been occurring with researchers in the Sensors and Electron Devices Directorate at ARL (Dr. Sina Najmaei and Dr. Adam Wilson). Several joint conference papers and joint archival papers are currently in preparation but none are expected to appear before 2019.

Dr. Najmaei is also an (unfunded) co-PI on a proposal that has been submitted to NSF on follow-on work to build the actual device whose design was enabled by the code written from this effort.

### PARTICIPANTS:

**Participant Type:** PD/PI

**Participant:** Peter W. Chung

**Person Months Worked:** 1.00

**Funding Support:**

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as of 03-Jan-2019

Project Contribution:  
International Collaboration:  
International Travel:  
National Academy Member: N  
Other Collaborators:

**Participant Type:** Graduate Student (research assistant)

**Participant:** Francis G. VanGessel

**Person Months Worked:** 6.00

**Funding Support:**

Project Contribution:  
International Collaboration:  
International Travel:  
National Academy Member: N  
Other Collaborators:

**Participant Type:** Undergraduate Student

**Participant:** Efreem Perry

**Person Months Worked:** 4.00

**Funding Support:**

Project Contribution:  
International Collaboration:  
International Travel:  
National Academy Member: N  
Other Collaborators:

**Participant Type:** Graduate Student (research assistant)

**Participant:** Jie Peng

**Person Months Worked:** 6.00

**Funding Support:**

Project Contribution:  
International Collaboration:  
International Travel:  
National Academy Member: N  
Other Collaborators:

**Participant Type:** Undergraduate Student

**Participant:** Mark Butrico

**Person Months Worked:** 2.00

**Funding Support:**

Project Contribution:  
International Collaboration:  
International Travel:  
National Academy Member: N  
Other Collaborators:

**Participant Type:** Postdoctoral (scholar, fellow or other postdoctoral position)

**Participant:** Abdollah Bagheri

**Person Months Worked:** 5.00

**Funding Support:**

Project Contribution:  
International Collaboration:  
International Travel:  
National Academy Member: N  
Other Collaborators:

**Participant Type:** Postdoctoral (scholar, fellow or other postdoctoral position)

**Participant:** Daniel C Elton

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**Person Months Worked:** 1.00

**Funding Support:**

Project Contribution:  
International Collaboration:  
International Travel:  
National Academy Member: N  
Other Collaborators:

**Participant Type:** Graduate Student (research assistant)

**Participant:** Gaurav Kumar

**Person Months Worked:** 9.00

**Funding Support:**

Project Contribution:  
International Collaboration:  
International Travel:  
National Academy Member: N  
Other Collaborators:

**CONFERENCE PAPERS:**

**Publication Type:** Conference Paper or Presentation

**Publication Status:** 1-Published

**Conference Name:** ASME 2015 International Mechanical Engineering Congress & Exposition

Date Received: 26-Aug-2016      Conference Date: 14-Nov-2015      Date Published: 14-Nov-2015

Conference Location: Houston, TX

**Paper Title:** Full-Band Microscale Heat Transfer Study of Fin Field Effect Transistor (FinFET) Designs

**Authors:** Francis G VanGessel, Peter W. Chung

Acknowledged Federal Support: **Y**

**Publication Type:** Conference Paper or Presentation

**Publication Status:** 1-Published

**Conference Name:** American Physical Society Spring Meeting

Date Received: 26-Aug-2016      Conference Date: 14-Mar-2016      Date Published: 14-Mar-2016

Conference Location: Baltimore, MD

**Paper Title:** Computational study of electronic and phonon properties of folded molybdenum disulphide (MoS<sub>2</sub>)

**Authors:** Jie Peng, Peter W. Chung

Acknowledged Federal Support: **Y**

**Publication Type:** Conference Paper or Presentation

**Publication Status:** 1-Published

**Conference Name:** American Physical Society Spring Meeting

Date Received: 26-Aug-2016      Conference Date: 14-Mar-2016      Date Published: 14-Mar-2016

Conference Location: Baltimore, MD

**Paper Title:** Scalable, Composable Operators for Defect Analysis and Design

**Authors:** Rose Weisburgh, Peter W. Chung

Acknowledged Federal Support: **Y**

**Publication Type:** Conference Paper or Presentation

**Publication Status:** 1-Published

**Conference Name:** Society for Engineering Science

Date Received: 30-Jan-2017      Conference Date: 05-Oct-2016      Date Published: 30-Jan-2017

Conference Location: College Park, MD

**Paper Title:** Electrical and thermal transport in the folds of MoS<sub>2</sub>

**Authors:** Jie Peng, Peter W. Chung

Acknowledged Federal Support: **Y**

**RPPR Final Report**  
as of 03-Jan-2019

**Publication Type:** Conference Paper or Presentation **Publication Status:** 1-Published  
**Conference Name:** Society for Engineering Science  
Date Received: 30-Jan-2017 Conference Date: 05-Oct-2016 Date Published: 30-Jan-2017  
Conference Location: College Park, MD  
**Paper Title:** Anisotropic Thermal Flow from the Full Brillouin Zone Solution to the Three Dimensional Phonon BTE  
**Authors:** Francis G. VanGessel, Peter W. Chung  
Acknowledged Federal Support: **Y**

**Publication Type:** Conference Paper or Presentation **Publication Status:** 1-Published  
**Conference Name:** Society for Engineering Science  
Date Received: 30-Jan-2017 Conference Date: 04-Oct-2016 Date Published: 30-Jan-2017  
Conference Location: College Park, MD  
**Paper Title:** Linear Operators for Spectral Analysis and Design  
**Authors:** Rose Weisburgh, Peter W. Chung  
Acknowledged Federal Support: **Y**

**Publication Type:** Conference Paper or Presentation **Publication Status:** 1-Published  
**Conference Name:** ASME International Mechanical Engineering Congress and Expo  
Date Received: 30-Jan-2017 Conference Date: 14-Nov-2016 Date Published: 30-Jan-2017  
Conference Location: Phoenix, AZ  
**Paper Title:** Full-Band Microscale Heat Transfer Study of Fin Field Effect Transistor (FinFET) Designs  
**Authors:** Francis VanGessel, Peter W. Chung  
Acknowledged Federal Support: **Y**

**Publication Type:** Conference Paper or Presentation **Publication Status:** 1-Published  
**Conference Name:** ASME International Mechanical Engineering Congress and Expo  
Date Received: 30-Jan-2017 Conference Date: 14-Nov-2016 Date Published: 30-Jan-2017  
Conference Location: Phoenix, AZ  
**Paper Title:** Linear Operators for Spectral Analysis and Design  
**Authors:** Rose Weisburgh, Peter W. Chung  
Acknowledged Federal Support: **Y**

**Publication Type:** Conference Paper or Presentation **Publication Status:** 1-Published  
**Conference Name:** ASME International Mechanical Engineering Congress and Expo  
Date Received: 30-Jan-2017 Conference Date: 14-Nov-2016 Date Published: 30-Jan-2017  
Conference Location: Phoenix, AZ  
**Paper Title:** Computational study of thermal and electronic transport in folded molybdenum disulphide nanostructure  
**Authors:** Jie Peng, Peter W. Chung  
Acknowledged Federal Support: **Y**

**Publication Type:** Conference Paper or Presentation **Publication Status:** 1-Published  
**Conference Name:** US National Congress in Computational Mechanics  
Date Received: 25-Aug-2017 Conference Date: 19-Jul-2017 Date Published: 19-Jul-2017  
Conference Location: Montreal, Quebec, Canada  
**Paper Title:** Lattice-Microscale Model to Determine Anisotropic Phonons & Thermal Conductivity in Molecular Crystal RDX  
**Authors:** Francis G. VanGessel, Peter W. Chung  
Acknowledged Federal Support: **Y**

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**Publication Type:** Conference Paper or Presentation **Publication Status:** 1-Published  
**Conference Name:** TMS 2018  
Date Received: 13-Jun-2018 Conference Date: 12-Mar-2018 Date Published: 11-Mar-2018  
Conference Location: Phoenix, Arizona  
**Paper Title:** Computational Phonon Manipulation  
**Authors:** Peter W. Chung  
Acknowledged Federal Support: **Y**

**Publication Type:** Conference Paper or Presentation **Publication Status:** 1-Published  
**Conference Name:** International Detonation Symposium  
Date Received: 29-Dec-2018 Conference Date: 16-Jul-2018 Date Published:  
Conference Location: Cambridge, Maryland  
**Paper Title:** A Phonon Boltzmann Study of Microscale Thermal Transport in alpha-RDX Cook-Off  
**Authors:** Francis G. VanGessel, Gaurav Kumar, Daniel C. Elton, and Peter W. Chung  
Acknowledged Federal Support: **Y**

**Publication Type:** Conference Paper or Presentation **Publication Status:** 1-Published  
**Conference Name:** Materials Research Society Fall Meeting and Exhibit  
Date Received: 13-Jun-2018 Conference Date: 26-Nov-2017 Date Published: 26-Nov-2017  
Conference Location: Boston, Massachusetts  
**Paper Title:** Tuning the electronic and thermal properties of SLMoS2 by folding  
**Authors:** Jie Peng and Peter W. Chung  
Acknowledged Federal Support: **Y**

**Publication Type:** Conference Paper or Presentation **Publication Status:** 1-Published  
**Conference Name:** ASME International Mechanical Engineering Congress & Exposition  
Date Received: 25-Oct-2018 Conference Date: 04-Nov-2017 Date Published: 04-Nov-2017  
Conference Location: Tampa, Florida  
**Paper Title:** Full Brillouin Zone BTE Model to Determine Anisotropic Phonos & Thermal Conductivity in Molecular Crystal RDX  
**Authors:** Francis G. VanGessel and Peter W. Chung  
Acknowledged Federal Support: **Y**

**Publication Type:** Conference Paper or Presentation **Publication Status:** 1-Published  
**Conference Name:** ASME International Mechanical Engineering Congress & Exposition  
Date Received: 13-Jun-2018 Conference Date: 03-Nov-2017 Date Published: 03-Nov-2017  
Conference Location: Tampa, Florida  
**Paper Title:** Tuning the electrical and thermal properties of folded SLMoS2  
**Authors:** Jie Peng and Peter W. Chung  
Acknowledged Federal Support: **Y**

**Publication Type:** Conference Paper or Presentation **Publication Status:** 1-Published  
**Conference Name:** World Congress in Computational Mechanics  
Date Received: 29-Dec-2018 Conference Date: 23-Jul-2018 Date Published:  
Conference Location: New York City, NY  
**Paper Title:** Atomic-Microscale Modeling of Phonons in the Molecular Crystal RDX Using Accurate Phonon Lifetimes  
**Authors:** Francis VanGessel, Gaurav Kumar, Daniel Elton, Peter W. Chung  
Acknowledged Federal Support: **Y**

**RPPR Final Report**  
as of 03-Jan-2019

**Publication Type:** Conference Paper or Presentation **Publication Status:** 2-Awaiting Publical  
**Conference Name:** Material Research Society Spring Symposium  
Date Received: Conference Date: 18-Apr-2019 Date Published:  
Conference Location: Phoenix, AZ  
**Paper Title:** Phonon Lifetimes in the Molecular Crystal alpha-RDX  
**Authors:** Gaurav Kumar, Francis VanGessel, Peter W. Chung  
Acknowledged Federal Support: **Y**

**Publication Type:** Conference Paper or Presentation **Publication Status:** 2-Awaiting Publical  
**Conference Name:** Americal Physical Society March Meeting 2019  
Date Received: Conference Date: 05-Mar-2019 Date Published:  
Conference Location: Boston, MA  
**Paper Title:** Phonones and thermal transport in hafnium disulphide (HfS<sub>2</sub>)  
**Authors:** Jie Peng, Peter W. Chung  
Acknowledged Federal Support: **Y**

**DISSERTATIONS:**

**Publication Type:** Thesis or Dissertation  
**Institution:** University of Maryland  
Date Received: 26-Aug-2016 Completion Date: 9/7/16 6:39PM  
**Title:** SCALABLE, COMPOSABLE OPERATORS FOR DEFECT DESIGN AND ANALYSIS  
**Authors:** Rose Weisburgh  
Acknowledged Federal Support: **Y**

**Publication Type:** Thesis or Dissertation  
**Institution:** University of Maryland  
Date Received: 26-Aug-2016 Completion Date: 4/12/16 6:39PM  
**Title:** Fully Anisotropic Solution of Three Dimensional Boltzmann Transport Equation  
**Authors:** Francis G. VanGessel  
Acknowledged Federal Support: **Y**

**Publication Type:** Thesis or Dissertation  
**Institution:** University of Maryland  
Date Received: 02-Jan-2019 Completion Date: 12/19/18 9:28PM  
**Title:** Phonon Modeling in Crystalline Materials  
**Authors:** Francis G. VanGessel  
Acknowledged Federal Support: **Y**

Nothing to report in the uploaded pdf (see accomplishments)