



Michigan Technological University

Department of Mechanical Engineering – Engineering Mechanics

Richard and Elizabeth Henes Professor of
Computational Mechanics

2019 Annual Report

Gregory M. Odegard

October 10, 2019

Introduction

The purpose of this report is to detail the research activities that were performed with support from the endowed position titled “Richard and Elizabeth Henes Professor of Computational Mechanics”. This position has been held since 2014 by Prof. Gregory M. Odegard of the Department of Mechanical Engineering – Engineering Mechanics (MEEM) at Michigan Technological University. Prof. Odegard is the Director of Research in the department, The director of the NASA Space Technology Research Institute (STRI) for Ultra-Strong Composite Materials by Computational Design (US-COMP), and the Site Director for the NSF supported Industry/University Collaborative Research Center (I/UCRC) on Novel High Voltage/Temperature Materials and Structures (NVT).

Prof. Odegard would sincerely like to thank the Henes family for their generous gift. Their continuous support for the MEEM department has made a difference in raising our profile among ME department around the country and has played an important role in improving the educational experience of both undergraduate and graduate students in our department.

Supported students

Between September 2018 and October 2019, the funds generated by this endowment were used to support MEEM PhD students and Hashim Al Mahmud and Khatereh Kashmari. Hashim is partially supported by a fellowship from the Iraq government to study in the U.S. Some of the Henes funds have been used to augment his government support so that he complete his work. He is a very dedicated, hard-working student and is worthy of this support.

Khatereh is partially supported by TA/grading assignments in MEEM and the Department at Physics at MTU. However, these funds are not enough to support her as a full-time PhD student. Thus I have used some of the Henes funds to augment this support. Like Hashim, Khatereh is hard working and has the potential to make an impact in her research area, and is thus worthy of the Henes support.

Resulting research accomplishments

Hashim’s research

During the time period between September 2018 and October 2019, Hashim conducted research on the molecular simulation of epoxy/GNP composites. This work is focused on finding epoxy-based nanocomposite materials with improved mechanical properties (strength, stiffness) relative to traditional composites. This is important for aerospace applications in which lightweight material need to be used that are resistant to high loads. Hashim’s work is a follow-on to the research of Cameron Hadden, a PhD student who graduated from our group a few years ago. Hashim is adding an important level of complexity to Cameron’s results. Whereas

Cameron only considered small mechanical deformations (elastic regime), Hashim's work is exploring the mechanical failure of these materials. This requires the use of a non-linear atomic potential, which is a mathematical relationship that describes the forces between atoms as a function of inter-atomic distance.

Hashim has successfully built computational models of the material and simulated the results. His work has shown that the nonlinear atomic potential (ReaxFF) works very well to predict the mechanical properties of these materials. He has shown this by comparison with our previous experiments on this material. In the future, these results will allow us to make more powerful and accurate predictions of material behavior for designing aerospace structures. Hashim will give a presentation at the 2020 ASCE (American Society of Civil Engineers) Earth and Space Conference in Seattle, WA in April 2020. He published his first journal article in this time period:

Al Mahmud, H., M.S. Radue, S. Chinkanjanarot, W.A. Pisani, Gowtham S., G.M. Odegard, "Multiscale Modeling of Carbon Fiber- Graphene Nanoplatelet-Epoxy Hybrid Composites Using a Reactive Force Field", *Composites Part B: Engineering*, Vol. 172, pp. 628-635 (2019)

He is working on a second manuscript that will be submitted for publication sometime in the next few months.

Khatereh's research

Khatereh's project is on a newer field of research known as process modeling. The goal of this work is to use computational modeling to optimize composite processing conditions to yield composite components with high levels of strength. Specifically, we use molecular modeling to determine the thermo-mechanical properties of composite materials on the molecular level as a function of processing time. This information is used in further simulations to predict the strength of composite structures. This research is being performed in conjunction with our partners at the University of Massachusetts at Lowell.

Khatereh's specific task in this project is to use molecular simulations to model the high-performance polymer poly-ether-ether-ketone (PEEK). This polymer is used in many aerospace and other demanding engineering applications. This system is very different than any that have been modelled in the past in this manner. Thus, her work is important in determining a modeling method that is suitable for thermoplastic resins. The goal is for her results to eventually lead to improvements in the mechanical performance of PEEK-based composite materials in the future.

Please don't hesitate to contact Prof. Odegard with any questions that you may have regarding this research or the use of the endowment funds. It is hoped that we can put this gift to use in the best possible way to facilitate our department's growth in research to be more globally competitive.