DEPARMENT OF MECHANICAL AND MATERIALS ENGINEERING
COLLEGE OF ENGINEERING AND APPLIED SCIENCE

SUMMER RESEARCH OPPORTUNITIES FOR UNDERGRADUATE WOMEN

APPLICATION DEADLINE: 03/01/2021

PROJECT TITLE: <u>Computer simulations of novel materials systems on atomic-length scales</u>

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Project Description

1. Area of research
With the advancement of high-performance computing and numerical methodologies, simulations have become an indispensable tool to investigate various physico-mechanical phenomena. In particular, atomistic simulations where material systems are explicitly modeled with discrete atoms interacting with one another have led to an improved understanding of the fundamental mechanisms underlying various material behaviors and properties. For example, molecular dynamics (MD), which is one of the most popular and powerful atomistic simulation tools, can provide the positions and momenta of all atoms at all instances of simulated time interval, which is not possible in experiments. This information, in turn, can be used to better understand the underlying mechanisms of observed physical phenomena. This route of research has proven to be very effective and productive in studying materials behaviors and properties from the fundamental level.

2. Research tasks the student will be performing
The student will construct computer models for atomistic systems and perform MD simulations using LAMMPS, a popular atomistic simulation tool developed at Sandia National Lab. The student will also analyze the simulation data using post-processing tools such as OVITO, VMD. In particular, the student will be involved in one of the following NSF-funded projects.

[Project 1] Friction of graphene
Graphite is a popular solid lubricant because its lamellar structure and weak interaction between layers provide low sliding resistance. In this respect, graphene, one-atom-thick graphite, is an ideal solid lubricant for MEMS

lubrication. Indeed, a number of studies have shown that graphene can reduce friction and wear at both nano and micrometer length scales. The objective in this research is to use atomistic computer simulations to study tribological properties of polycrystalline graphene.

[Project 2] Brittle-to-ductile transition of silicon
Silicon is the most commonly used semiconductor material and has played a critical role in the recent advances in nanotechnology as a building material for MEMS (micro-electro-mechanical systems). Silicon on small length scales often exhibits completely different behaviors from its bulk counterparts and one of the most important size-dependent properties is the brittle-to-ductile transition (BDT), that is, brittle silicon becomes ductile above a critical temperature. The plastic deformation of silicon has a profound impact on the reliability of MEMS as the applied loads and operating conditions become more severe. Also, due to the brittle fracture, silicon-based structures cannot be machined, but should be fabricated in a variety of artful ways. In recent years, several experiments have found that silicon-based structures on sub-micrometer scales exhibit plastic deformation even at room temperature. However, our current understanding of the size-dependent BDT phenomenon of silicon still remains far from complete and it is not rare to find that experimental observations are contradictory to each other and reasonable explanations are not provided. In this research, we plan to study the size-dependent BDT of single-crystal silicon using atomistic simulations.

[Project 3] Nanoscale cutting of ceramic materials
Ceramic materials have found various applications, especially under harsh conditions, thanks to their superior mechanical, electrical, optical, chemical, thermal, and biocompatible properties. However, since ceramics shatter upon impact rather than deform, manufacturing ceramic devices of complex shapes and high-quality surfaces is a challenge. Ultra-precision machining of ceramics has found a way to overcome this challenge by cutting or removing very tiny amounts of material. However, its productivity is not satisfactory and an understanding of the material behavior under cutting, especially at atomic scale, remains elusive. This project is to find optimized machining conditions for ceramic materials based on an improved understanding of material failure. This understanding is obtained by a combined strategy of state-of-the-art experiment and atomistic simulation approaches coupled with machine learning algorithms. This approach facilitates the machining of advanced ceramics without the need for extra post-processing, which is expensive and time consuming and, thus, achieves industry-required productivity. Moreover, by improving the fabrication process and damage control of ceramic materials, high quality ceramic components such as engine blocks, camera lenses, high energy lasers, and biomedical implants are possible, which benefits U.S. industry and economy. This award engages students from historically underrepresented groups in research experiences, leveraging Graduate Engineering Research Scholar and Women in Science and Engineering Programs.

3. Training that the mentor will provide to the WISE student
In addition to LAMMPS and OVITO, the student will learn basic computer skills

(Linux, parallel computing) and some theoretical background knowledge (e.g. multi-body dynamics, statistical mechanics, numerical methods, etc.) that are needed to perform atomistic simulations. The student will cowork with a graduate student who can help the student to conduct this research. The student will also be invited to join our group's weekly meeting where graduate students give a talk about their research areas.

4. Specific requirements:
There is no specific requirement, but the following skills and knowledge will be helpful; computer programing, parallel computing, Linux operating system.