MECHANICAL AND MATERIALS ENGINEERING
COLLEGE OF ENGINEERING AND APPLIED SCIENCE

SUMMER RESEARCH OPPORTUNITIES FOR UNDERGRADUATE WOMEN

APPLICATION DEADLINE: 03/01/2020

PROJECT TITLE: <u>Molecular dynamics simulation for graphene friction</u>

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Project Description

1. Area of research
Friction of machine parts in sliding contact is a primary cause of significant energy loss, which has a great impact on the sustainability of human civilization. For example, a conservative study estimated that 1.3 -1.6 % of an industrialized nation's GDP is lost due to friction and wear of mechanical parts. On macroscopic scales various means of lubrication including both solid and fluid lubricants can be used for sliding surfaces. However, solid lubrication through coating may be the only viable technique of lubrication for small length-scale devices such as MEMS (micro-electro-mechanical-systems) because fluid lubricants applied to such devices can cause excessive loss of power. Thus, significant research efforts have been made to develop effective lubricant materials that can be used on microscopic scales for a wide range of MEMS applications. 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. There are other types of 2-D materials, which share the superior tribological properties with graphene such as h-BN, MoS_2, etc. Furthermore, graphene layers have been known to possess an extraordinary property called superlubricity, i.e., friction between two graphene layers becomes vanishingly small under some conditions (e.g. incommensurate interfaces exhibit superlubricity as shown in the figure). The objective in this research is to use atomistic computer simulations to study tribological properties of polycrystalline graphene.
2. Research tasks the student will be performing

The student will construct computer models for 2-D materials such as graphene and h-BN and perform computer 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.

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.