

STATEMENT OF PURPOSE

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Innovative nanostructured materials have attracted extensive scientific interest due to their unique thermal properties. For traditional bulk materials, we cannot alter their thermal properties significantly. But at nanoscale, we can tune and even break the limit of thermal properties of materials. Nano-materials actually give us a far better chance to produce next generation of thermoelectric devices to resolve energy shortage problems. Current energy conversion efficiency of these devices is not satisfying for commercial uses due to the lack of a detailed understanding of thermal transport in nanostructures. Thus I am desirous to conduct research on nanoscale thermal transport, especially on phonon transport and phonon manipulation during my PhD studies to bring us closer to that bright future.

My undergraduate study has strengthened my skills and knowledge to study thermal transport. My major courses such as thermodynamics (91/100), heat transfer (96/100) and fluid dynamics (99/100) helped me to understand basic rules and principles of energy conversion and thermal management. Meanwhile, I acquired solid skills in coding for high precision scientific computation from the course of numerical methods (100/100) and C++ programming design (95/100). In Nano Heat Group led by Prof. Nuo Yang, I obtained further knowledge of mechanism of nanoscale thermal transport.

My research experience in Nano Heat Group taught me how to come up with novel ideas to picture and investigate transport phenomena via programming and developed my ability of critical thinking. I focused on finding ways to reduce thermal conductivity of graphene for its potential thermoelectric application. Folding has been proved to be a useful way to manipulate the thermal conductivity of graphene nanoribbon. However, given the fact that there exists a strong size effect on thermal conductivity of graphene, the large-area folded graphene may be a different case and thus should be investigated. I successfully applied my own FORTRAN program to set atom's initial position, initial velocity distribution and atom reciprocal potentials explicitly and reasonably. To obtain an size-independent thermal conductivity characterizing large-area graphene, a series of simulation cases were calculated. Challenging was that computers cannot deal with some cases of extremely large simulation scale. I subtly optimized the code to accelerate the computing process and solved this issue successfully. And my results clearly show that thermal conductivity decreases significantly with increasing number of folds and stronger substrate effect, caused by the enhanced phonon scattering. This proves that even for large-area graphene with folds, folding still greatly contributes to reducing the thermal conductivity. This work is being enriched and will be published soon. From this work, I learned every detail of MD simulation and gained great pleasure from integrating my thoughts and efforts into efficient solutions to crack puzzles in the amazing nano world.

Besides, capability of collaboration helped me more prepared for my future research. In the research on coupling between different phonon modes in graphene, doctoral candidate Meng An came up with theory model and I built the simulation model to verify its validity. Then we discussed how to modify the model based on simulation results. We did this feedback process time after time for months to make sure we finally obtained an appropriate model that can rationally quantify coupling strength. Meanwhile, we kept doing double-check of each other's work to prevent mistakes. It was teamwork that inspired me constantly and promoted the research greatly.

With my strong background, I believe I am well prepared to attend graduate school and contribute to the field of nanoscale thermal transport. I seek advanced knowledge and skills I need from the graduate program to systematically conduct my research. The Department of Mechanical Engineering at University of Colorado Boulder is known for its advanced interdisciplinary studies, especially in nano-systems and energy engineering. It will be a precious experience for me to conduct cutting-edge research and learn how to innovate in face of challenges during my PhD studies. After my graduation, I will definitely keep pursuing my academic career in the area of nanoscale heat transfer for I believe that Rome was not built in one day: to convert my expertise into valuable scientific and social contribution, years of continuous effort is a must.