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Department of Mechanical Engineering

Design Robust and Highly Efficient Thermoelectric Materials through Microstructure, and Light Irradiation

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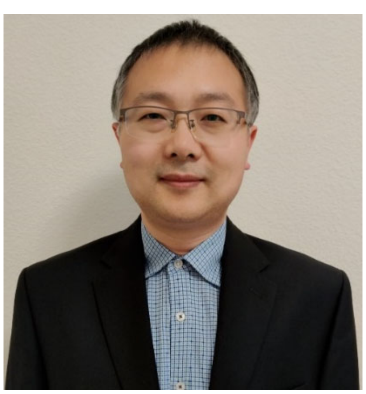
Overconsumption of fuel oils and the resulting energy crisis have been increasingly causing environmental issues such as global climate change and marine pollution. Solid-state thermoelectric (TE) technology, enabling direct conversion between heat and electricity without moving parts, offers the possibility for relieving the current energy crisis. The widespread application of TE technology requires TE materials with high conversion efficiency and robust mechanical properties. However, it has been challenging to develop highly stable and efficient TE materials in expensive and time-consuming experiments. Computer simulations may dramatically accelerate the design of novel TE materials with desirable properties. In this talk, we illustrate how to improve the mechanical properties and efficiency of TE materials via microstructure engineering and light irradiation via an AI-based theoretical framework including machine learning, quantum mechanics, and atomistic simulations. First, we show that the strength of both InSb and Bi_2Te_3 can be significantly enhanced due to the nanoscale twins. For Bi_2Te_3, the strengthening mechanism is due to the formation of twin boundaries between the Te atoms of adjacent Te1─Bi─Te2─Bi─Te1 quint substructures. For InSb, it arises from the directional covalent bond rearrangements at the twin boundary accommodating the structural mismatch. Then we show that the lattice thermal conductivity (LTC) of Mg_2Si can be significantly reduced due to the light irradiation and nanoscale twins, which increases the conversion efficiency between heat and electricity. The light irradiation causes the different distributions of excess electrons and holes under e–h excitation, leading to softening phonon modes. The nanotwins cause the rattling of Mg□Mg bond along TBs, leading to soft acoustic and optical modes, shorter phonon lifetime, and higher phonon scattering rate. Finally, we report the decreased LTC of high temperature TE material boron subphosphide ($B_{12}P_2$) by introducing the nanoscale twins. The decrease of vibrational density of states and phonon participation ratio due to TBs' phonon scattering is the main reason of the low LTC in nanotwinned $B_{12}P_2$. The new knowledge gained in this talk is important for the future design of novel TE materials with designed properties via controlling microstructures and light irradiation.



Bio Sketch

Dr. Qi An is an Assistant Professor in Materials Science at the University of Nevada, Reno (UNR). He received his MS and PhD degrees in Materials Science from Caltech, and his BS degree from the University of Science and Technology of China. His research area is computational materials science covering machine learning, electronic structure calculations and atomistic simulations. His research specifically focuses on mechanical properties of superhard ceramics, semiconductors, and thermoelectric materials; computational materials design; metallic glasses; material behaviours under extreme conditions; and heterogeneous catalysis. He has authored or co-authored about 170 publications in scientific journals

Department of Mechanical Engineering, Edward E. Whitacre Jr. College of Engineering

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In person: ME South 205

Online:
https://texastech.zoom.us/j/94591486607?pwd=MHhsSnJyM2RJQjl1ZmdsWkZuVExrQT09
Meeting ID: 945 9148 6607
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