NUS National University of Singapore

Department of Materials Science and Engineering Seminar Series 2025

STUDIES OF LOW-DIMENSIONAL STRUCTURES AND THEIR IMPACT ON PROPERTIES IN THERMOELECTRIC MATERIALS BY TRANSMISSION ELECTRON MICROSCOPY

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Date and time: July the 17th (Thursday) at 10am

Venue: E3-06-08

Abstract

Low-dimensional structures play a critical role in the properties of thermoelectric materials, yet the atomic-level mechanisms remain poorly understood. Here, we employ ultrafast electron diffraction with both high temporal and spatial resolution to probe local Ag^+ structures in the superionic conductor $AgCrSe_2$ and elucidate the complete diffusion process. Our findings indicate that the process originates from localized Ag^+ vibrations, followed by the formation of Ag^+ trimer structures through a rapid contraction of the Ag^+-Ag^+ bond from ~3.68 Å to ~3 Å over 1.97 picoseconds. Molecular dynamics simulations further demonstrate that these contracted local structures promote fast ion diffusion by opening up excess free volume and reducing local energy barriers. In the chain-like thermoelectric material InTe, a combination of selected area electron diffraction (SAED), scanning transmission electron microscopy (STEM), integrated differential phase contrast (iDPC) and theoretical calculations reveals spiral density waves of In^{1+} disorder chains, and a significant density of

vacancies at the In^+ sites along with indium interstitials. Variations in the concentration of In^+ interstitials trigger a transition from trivial conductivity to charge-density wave-like electrical conductivity at low temperatures. These findings provide new insights into the atomic-level mechanisms that govern ion diffusion and lattice thermal conductivity, offering pathways for the design of next-generation thermoelectric and superionic materials.

Biography

Yang Jianmin received her B.Eng. degree in Materials Science and Engineering from the Northeastern University in 2016 and M.Sc. degree from Beihang University in 2019. She is currently a Ph.D. candidate in the Department of Materials Science and Engineering under the supervision of Assoc. Prof. Michel Bosman. Her research focuses on the study of low-dimensional structures and their impact on the properties of thermoelectric materials by Transmission Electron Microscopy.

Please join us!

HOST: Asst. Prof He Qian