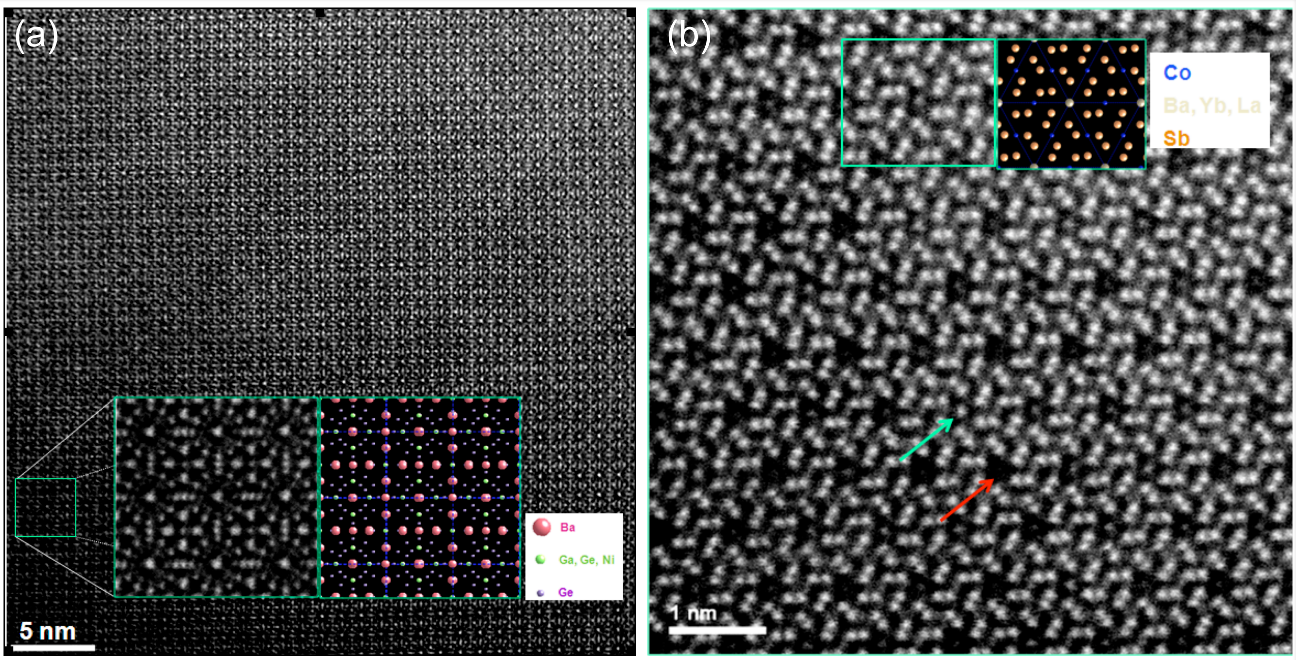
Study of the Microstructure of Doped Clathrate and Skutterudite Thermoelectric Materials

Jihui Yang, Xun Shi, General Motors
Hsin Wang and Miaofang Chi, Oak Ridge National Laboratory

Scientific challenge/problem: Clathrate and Skutterudite are known to be promising thermoelectric materials. The R&D groups at GM and ORNL have found that doping Clathrate ($Ba_{0.25}Co_4Sb_{12}$) with Yb and La and doping Skutterudite ($Ba_8Ga_{16}Ge_{30}$) with Ni improve the thermoelectrical properties significantly. The goal of the microscopy characterization is to fundamentally understand how the dopants control the materials properties. Two questions need to be answered at the current stage of our experimental work: how the microstructures are tailored by the dopants and how the dopants distribute in the materials.



(a) HAADF-STEM imaging shows that the Clathrate is perfectly uniform and no 2nd phase or nano-inclusions are observed in the grains or on the grain boundaries. A higher magnification HAADF-STEM image is inset and compared with the structure model for this material. (b) STEM-HAADF image shows that the atomic distribution of the dopants in the Skutterudite cages are not uniform, which is revealed by the contrast of the cage atom columns. Two examples are marked by arrows.

Accomplishment: The microstructure of Clathrate is extremely uniform, free of defects and second phases and nano-inclusions, and demonstrates a uniform distribution of dopants. This is probably the key feature to enhancing the thermoelectric properties of this material. Doping elements in Skutterudite are non-homogeneously distributed in the cages, which raises an interesting question about how much the thermoelectric properties can be further improved with a more ordered cage-filled structure. Further imaging and chemical analyses are planned determine greater detail regarding the distribution of La, Yb, and Ba.

SHaRE-HTML User Research Highlight