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The Atomic Structure of Ga and Ge in Ba-Ga-(Si,Ge) Clathrate
A.N. MANSOUR, NSWCCD, J.B. MARTIN, W. WONG-NG, NIST, G.S. NOLAS, USF — Compression studies on $Sr_8Ga_{16}Ge_{30}$ type I clathrate revealed a 3 fold increase in "ZT" [J. F. Meng et al., J. Appl. Phys., 89, 1730 (2001)]. Substitution of Si for Ge in Ba-Ga-Ge clathrate could mimic the effect of bulk compression, and subsequently enhance "ZT". Recent studies on Si substituted Ba-Ga-Ge clathrate have shown a decrease in the lattice constant and an increase in the power factor with Si substitution. However, the effects of Si on the electronic and local atomic structures of Ga and Ge have not been investigated in detail. We have used XAS to characterize the electronic and local atomic structures of Ga and Ge for a number of samples with varying degree of Si substitution. Analysis of Ga and Ge K-edge XANES spectra revealed that the partial density of p-states was modified for both Ga and Ge with Si substitution with the changes being more pronounced in the case of Ga. Comparisons of Fourier transforms of EXAFS spectra revealed that the local structure of Ga is significantly changed with Si substitution while changes in the local structure of Ge with Si substitution are moderate.

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