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Thermal conductance of graded silicon germanium superlattices SHUNDA CHEN, University of California Daivs, RUOCHONG SHEN, University of California Daivs, University of Zhejiang University, PABLO FERRANDO-VILLALBA, JAVIER RODRIGUEZ-VIEJO, Universitat Autnoma de Barcelona, DAVIDE DONADIO, University of California Daivs — Minimizing the thermal conductivity of silicon germanium (SiGe) superlattices is of interest for thermoelectric applications of Si-based devices [1]. Recent experiments have shown unprecedented control in the growth of SiGe superlattices with graded concentration profiles, in which dramatic reduction of the thermal conductance was observed [2]. In this work we use atomistic lattice dynamics simulations to understand the microscopic mechanisms leading to such reduction of the thermal conductance in graded SiGe superlattices. An efficient implementation of the elastic scattering formalism [3] allows us to compute the transmission function and the thermal conductance of atomistic models with the same system size scale as the experimental systems, and to explore the relation between the thermal conductance and the structural parameters of graded superlattices. The database of results thus acquired is analyzed using machine learning methods [4], so to devise a predictive model for thermal transport in this class of systems. [1] C.J. Vineis, et al., Adv. Mater. 22, 3970 (2010) [2] P. Ferrando-Villalba, et al., Nano Research 8(9),2833 (2015) [3] I. Duchemin, D. Donadio, Phys. Rev. B 84, 115423 (2011) [4] T. Hastie, et al., The Elements of Statistical Learning (Springer, 2009)

Shunda Chen
University of California Daivs

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