

# **Ultra-low Lattice Thermal Conductivity and Enhanced Thermoelectric Performance in SnTe:Ga Materials**

Rabih Al Rahal Al Orabi,<sup>\*,†,‡</sup> Junphil Hwang,<sup>¶</sup> Chan-Chieh Lin,<sup>§</sup> Régis Gautier,<sup>||</sup> Bruno Fontaine,<sup>||</sup> Woochul Kim,<sup>¶</sup> Jong-Soo Rhyee,<sup>§</sup> Daehyun Wee,<sup>†</sup> and Marco Fornari<sup>\*,⊥</sup>

*Department of Environmental Science and Engineering, Ewha Womans University, Seoul, 120-750, Korea, Department of Physics, Central Michigan University, Mt. Pleasant, MI 48859, USA , School of Mechanical Engineering, Yonsei University, Seoul, 120-749, Korea,*

*Department of Applied Physics, College of Applied Science, Kyung Hee University, Yongin-si, Giheung-gi, Gyeonggi-do 446-701, Korea, Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS-Université de Rennes 1-Ecole Nationale Supérieure de Chimie de Rennes, 11 allé de Beaulieu, CS 50837, F-35708 Rennes, France., and Department of Physics and Science of Advanced Materials Program, Central Michigan University, Mt. Pleasant, MI 48859, USA*

E-mail: alrah1r@cmich.edu; marco.fornari@cmich.edu

---

<sup>\*</sup>To whom correspondence should be addressed

<sup>†</sup>Department of Environmental Science and Engineering, Ewha Womans University, Seoul, 120-750, Korea

<sup>‡</sup>Department of Physics, Central Michigan University, Mt. Pleasant, MI 48859, USA

<sup>¶</sup>School of Mechanical Engineering, Yonsei University, Seoul, 120-749, Korea

<sup>§</sup>Department of Applied Physics, College of Applied Science, Kyung Hee University, Yongin-si, Giheung-gi, Gyeonggi-do 446-701, Korea

<sup>||</sup>Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS-Université de Rennes 1-Ecole Nationale Supérieure de Chimie de Rennes, 11 allé de Beaulieu, CS 50837, F-35708 Rennes, France.

<sup>⊥</sup>Department of Physics and Science of Advanced Materials Program, Central Michigan University, Mt.

## Supporting Information Available

We include the powder XRD patterns for  $\text{Sn}_{1.03-x}\text{Ga}_x\text{Te}$  ( $x = 0, 0.02, 0.03, 0.05, 0.07$  and  $0.09$ ) samples (Fig.1). Input parameters for the calculation based on the Klemens's model at 300 K are in Tab. 1. In Fig. 2a-c, we include the measurementes of the electrical conductivity, the Seebeck coefficients and the thermal diffusivity for 7% Ga-doping samples. The calculation of the Lorenz number as a function of concentration  $x$  for  $\text{Sn}_{1.03-x}\text{Ga}_x\text{Te}$  ( $x = 0, 0.02, 0.03, 0.05, 0.07$  and  $0.09$ ) and temperature is in Fig. 2d. Additional results from DFT are also included in Fig. 3: the electronic band structure of  $\text{Sn}_{32}\text{Te}_{32}$  and  $\text{Sn}_{30}\text{Ga}_2\text{Te}_{32}$  represeted for the cubic supercells.

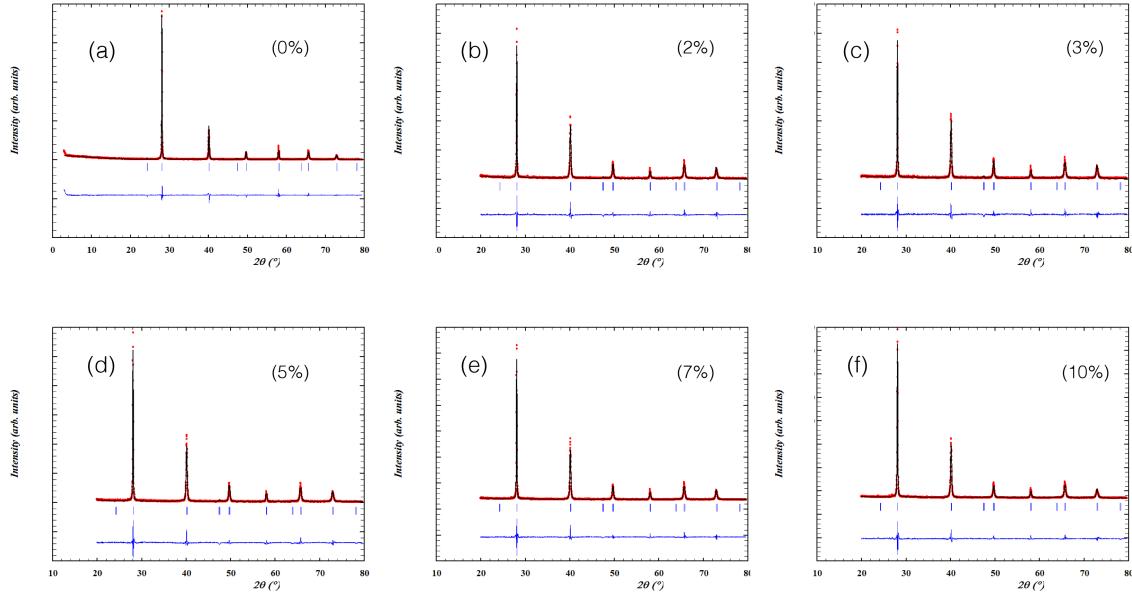


Figure 1: Powder XRD patterns for  $\text{Sn}_{1.03-x}\text{Ga}_x\text{Te}$  samples after hot pressing. Observed (red), calculated (black and vertical line bars) and difference plots (blue) shifted by a constant for clarity ( $\lambda = 1.5406 \text{ \AA}$ )

---

Pleasant, MI 48859, USA

Table 1: Input parameters for Klemens's model calculation at 300 K.

Grüneisen parameter <sup>1</sup> ( $\gamma$ )	Poisson ratio <sup>2</sup>	$\varepsilon$ (related to elastic properties) <sup>3,4</sup>
2.1	0.244	$\sim 163$
Debye temperature ( $\Theta_D$ ) <sup>5</sup>	average sound velocity <sup>6</sup> ( $v$ )	
$\sim 140$ K	$\sim 1800$ (m/s)	

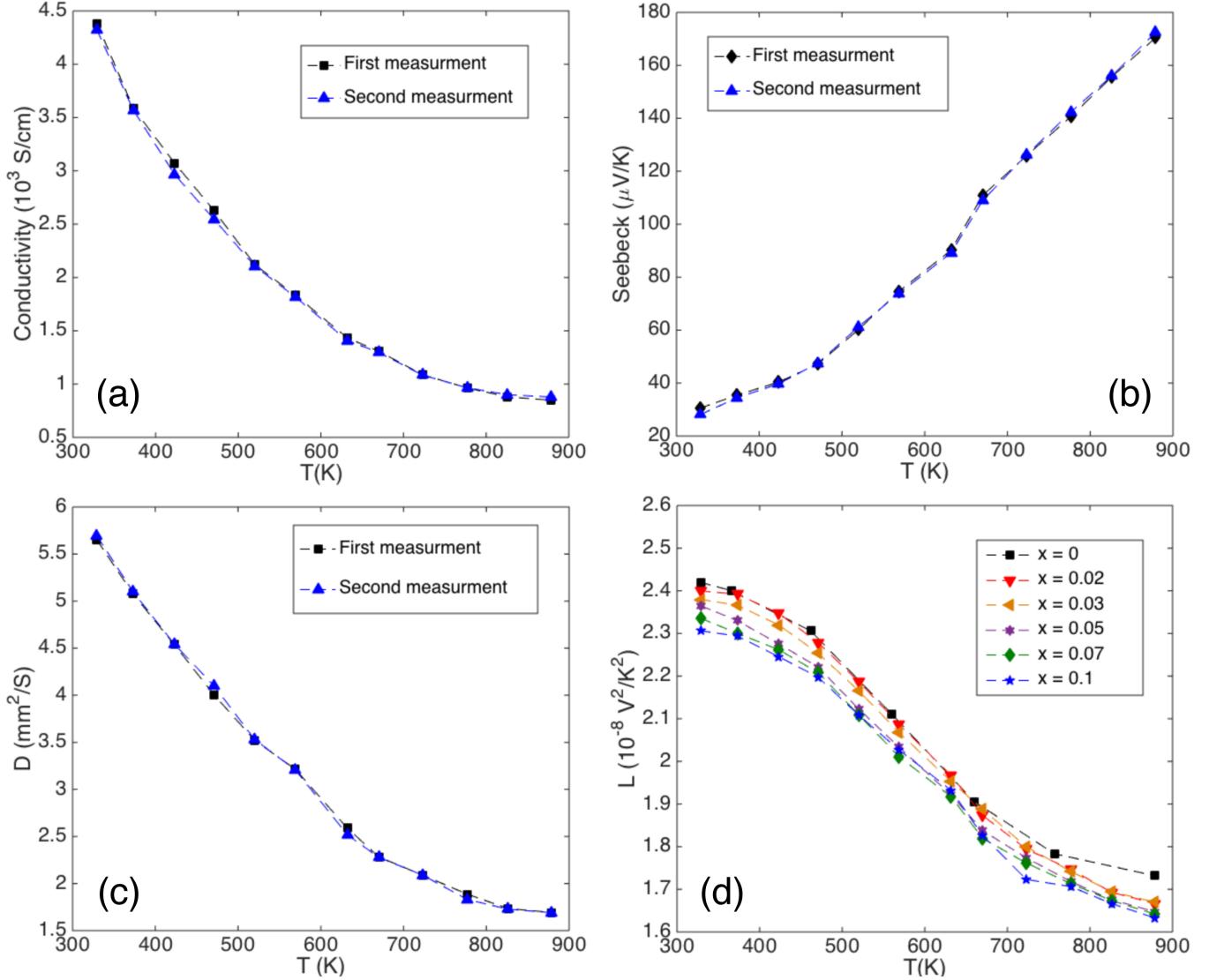


Figure 2: Temperature dependence of (a) electrical conductivity; (b) Seebeck coefficient; (c) thermal diffusivity for  $\text{Sn}_{0.94}\text{Ga}_{0.07}\text{Te}$  samples, (d) Lorenz number  $L$  as a function of temperature for  $\text{Sn}_{1.03-x}\text{Ga}_x\text{Te}$  samples

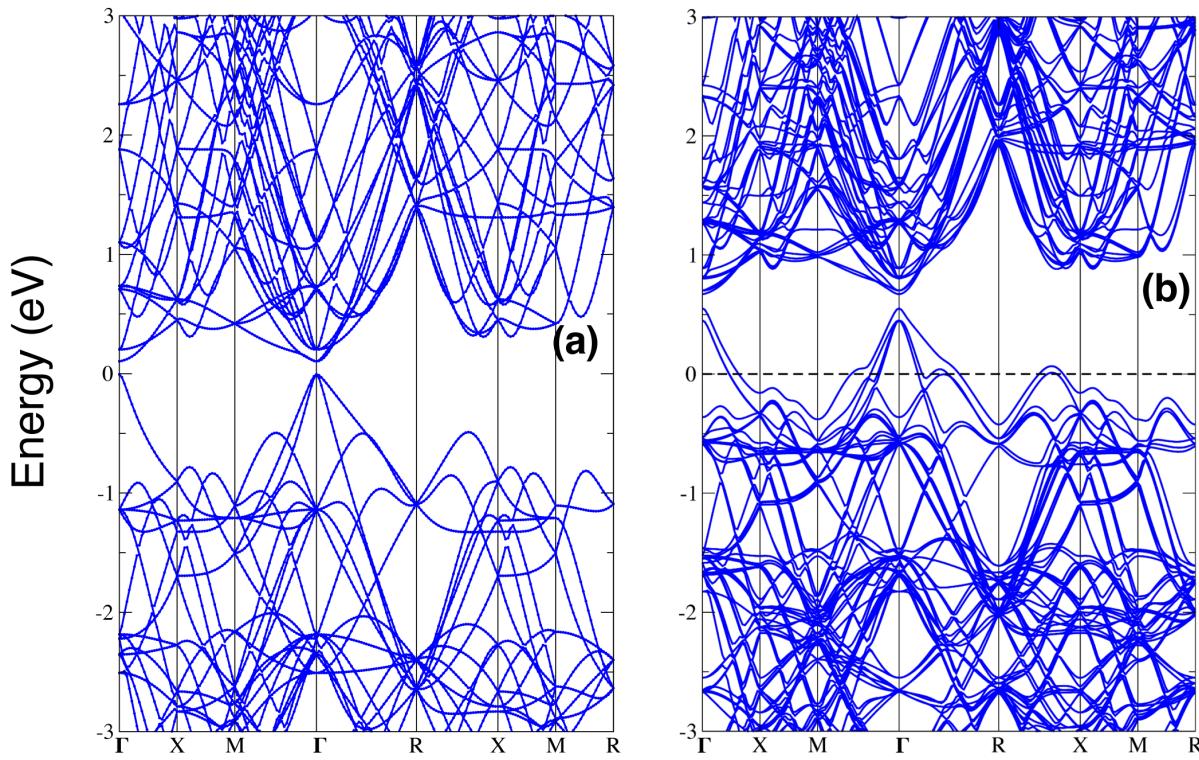


Figure 3: Electronic band structure calculation of  $\text{Sn}_{32}\text{Te}_{32}$  (a),  $\text{Sn}_{30}\text{Ga}_2\text{Te}_{32}$  (b) cubic supercells

This material is available free of charge via the Internet at <http://pubs.acs.org/>.

## References

- (1) Toher, C.; Plata, J. J.; Levy, O.; de Jong, M.; Asta, M.; Nardelli, M. B.; Curtarolo, S. High-Throughput Computational Screening of Thermal Conductivity, Debye Temperature, and Grüneisen Parameter Using a Quasiharmonic Debye Model. *Phys. Rev. B: Condens. Matter Mater. Phys.* **2014**, *90*, 174107.
- (2) Schmidt, R.; Case, E.; Ni, J.; Trejo, R.; Lara-Curzio, E.; Korkosz, R.; Kanatzidis, M. High-Temperature Elastic Moduli of Thermoelectric  $\text{SnTe}_{(1+x)}y\text{SiC}$  Nanoparticulate Composites. *J. Mater. Sci.* **2013**, *48*, 8244–8258.
- (3) Anderson, D. L.; Anderson, O. L. Lattice Thermal Conductivity of Disordered Semiconductor Alloys at High Temperatures. *J. Geophys. Res.* **1970**, *75*, 3494.

- (4) Anderson, O. L.; Nafe, J. E. Lattice Thermal Conductivity of Disordered Semiconductor Alloys at High Temperatures. *J. Geophys. Res.* **1965**, *70*, 3951.
- (5) Bukshpan, S. Determination of the Debye Temperature of SnTe Using the Massbauer Effect in <sup>119</sup>Sn and <sup>125</sup>Te. *Solid State Commun.* **1968**, *6*, 477 – 478.
- (6) Bauer Pereira, P.; Sergueev, I.; Gorsse, S.; Dadda, J.; Mller, E.; Hermann, R. P. Lattice Dynamics and Structure of GeTe, SnTe and PbTe. *phys. status solidi (B)* **2013**, *250*, 1300–1307.

# Graphical TOC Entry

