Electronic Supplementary Information

The phonon scattering mechanism and its effect on temperature dependent thermal and thermoelectric properties of the silver nanowire

Gui-Cang He,* Li-Na Shi, Yi-Lei Hua* and Xiao-Li Zhu*

Key Laboratory of Microelectronic Devices & Integrated Technology, Institute of Microelectronics, Chinese Academy of Sciences, Beijing 100029, P. R. China.

*E-mail: heguicang@163.com; huayilei@ime.ac.cn; xiaoli.zhu@sitrigroup.com.

1. The cross-section of AgNW

The cross section shape of AgNW is about triangle, which is measured at the three points along the AgNW. The average height (*h*) and full width at half maximum (*w*) of the cross section are 142 ± 5 nm and 367 ± 12 nm, respectively.

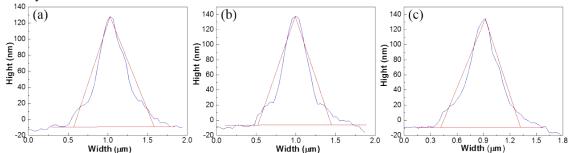


Figure S1. The cross section (blue curves) of the AgNW measured by AFM at the three points on the AgNW (a, b, c), and the triangles (red lines) is used to calculated the area of the cross section.

2. The temperature dependent resistances of the AgNW

In order to obtain the electrical resistivity and the Debye temperature of the AgNW, the electrical properties of the AgNW have to be investigated. The I-U curves of the AgNW is characterized using a Keilthley 4200-SCS semiconductor system with the CRX-4K Cryogenic probe station in vacuum environment. Two golden conical probes are placed to connect two electrical pads, and then an impressed voltage is applied to detect the corresponding current. The temperature variation range is between 10 and 300 K in the temperature dependence characterization. The resistances of the AgNW are obtained by the linear fitting of the I-U curves. Figure S2(a) and Fig. S2 (b) show the measured I-U curves and fitted lines of the AgNW at temperature of 10 K and 300 K, respectriviely. The temperature dependent resistances of AgNW can be investigated in the framework of the Boltzmann transport theory using Bloch-Grüneisen formula¹

$$R = R_0 + R_{el-ph},$$

$$R_{el-pl} = \partial_{el-ph} \left(\frac{T}{\theta_D}\right)^5 \int_0^{\theta_R/T} \frac{x^5}{(e^x - 1)(1 - e^x)} dx, \qquad (1)$$

where, R_0 is the residual resistance component, R_{el-ph} is the temperature dependent resistance component, which describes a scalar determining the electron-phonon coupling constant (α_{el-ph}), θ_D is the Debye temperature. Those parameters of the AgNW can be abstracted from the Bloch-Grüneisen formula fitting with resistances of the AgNW at different temperature (Fig. S2(c)).

Due to impurities and the structure defects scattering of electrons in AgNW,^{2,3} the residual resistivity of AgNW (8.12×10⁻⁸ Ω ·m) is about three orders of magnitude enhanced with respect to the corresponding bulk value (10⁻¹⁰ Ω ·m).¹ Both the electron-phonon coupling constant (5.60×10⁻⁸ Ω ·m) and the slope of the electrical resistivity (6.29×10⁻¹¹ Ω ·m·K⁻¹) of the AgNW against temperature are also larger than those of the corresponding bulk (5.24×10⁻⁸ Ω ·m, 6.11×10⁻¹¹ Ω ·m·K⁻¹).⁴ Because of the phonon softening (AgNW surface and internal twin boundaries scattering),^{5,6} the Debye temperature of the AgNW (223 K) is lower than that of the corresponding bulk (235 K).⁴ Here, the defect concentration ($R_0/(R-R_0)$)⁷ of the AgNW is 4.45, which should be considered in

the discussion of mass density and electron number density problems of the AgNW. Besides, the resistivity of the AgNW at room temperature is about $9.95 \times 10^{-8} \Omega \cdot m$, about 5 times of the corresponding bulk resistivity ($1.60 \times 10^{-8} \Omega \cdot m$). The resistivity of the AgNW is much lower than that of AgNW fabricated by other methods.^{8,9}

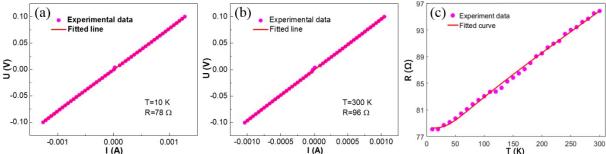


Figure S2. The measured I-U curves of the AgNW and fitted lines at temperature of (a) 10 K and (b) 300 K, (c) The temperature dependent resistances of the AgNW and fitted with the Bloch-Grüneisen formula.

3. The temperature dependent specific heat capacity of the AgNW and the bulk silver

The temperature dependent specific heat capacity variation trend of the AgNW is similar with that of the bulk silver (Fig. S3). However, the specific heat capacity of the AgNW is higher than that of the corresponding bulk when temperature is lower than 30 K, while it is lower than that of the bulk when the temperature is higher than 30 K. The reason for this phenomenon is that the specific heat capacity of the AgNW is considered only in one dimension, and that of the bulk silver is considered in three dimensions. Besides, the body size of the AgNPs in the AgNW enhances the specific heat capacity when the temperature is below 30 K.¹⁰

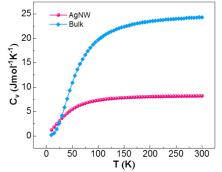


Figure S3. The temperature dependent specific heat capacity of the AgNW and the bulk silver.

4. Lattice thermal conductivity $\binom{k_L^u}{k_L^u}$ considering the phonon-phonon scattering process

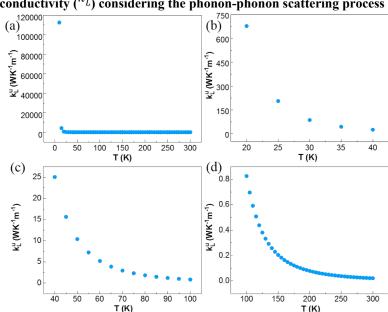


Figure S4. Lattice thermal conductivity considering the phonon-phonon scattering process in different temperature ranges, (a) 10-300 K, (b) 20-40 K, (c) 40-100 K, (d) 100-300 K.

The lattice thermal conductivity $\binom{k_L^u}{l}$ determining the phonon-phonon scattering process decreases with temperature, which decreases more and more slowly as the temperature increases (Fig. S4).

5. Lattice thermal conductivity $\binom{k_L^b}{k}$ considering the phonon structure scattering process

Since, the lattice thermal conductivity is related to the specific heat capacity of the material, the temperature dependent lattice thermal conductivity $\binom{k_L^b}{L}$ of AgNW considering phonon structure scattering is not constant, which increases with the temperature (Fig. S5).

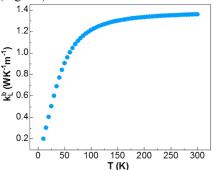


Figure S5. The lattice thermal conductivity of the AgNW considering the phonon structure scattering process.

6. The compatibility factor of the AgNW

As shown in Fig. S6, the compatibility factor (*S*) of the AgNW decreases with the temperature when it is below than 60 K. After that, the *S* increases with the temperature. However, the changed value of the *S* is only about 2.5×10^{-3} V⁻¹ in its operating temperature range. Obviously, the changed value of the factor with temperature is relatively small, which is very important for the stability of the thermoelectric device.

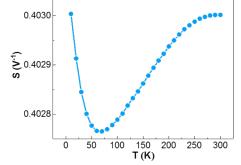


Figure S6. The temperature dependent compatibility factor of the AgNW.

REFERENCES

¹S. Kim, H. Suhl, and I. K. Schuller, Phys. Rev. Lett. 78, 322 (1997).

²E. J. Menke, M. A. Thompson, C. Xiang, L. C. Yang, and R. M. Penner, Nat. Mater. 5, 914 (2006).

³G. C. He, H. Lu, X. Z. Dong, Y. L. Zhang, J. Liu, C. Q. Xie, and Z. S. Zhao, RSC Adv. 8, 24893 (2018).

⁴Z. Cheng, L. J. Liu, S. Xu, M. Lu, and X. W. Wang, Sci. Rep. 5, 10718 (2015).

⁵D. R. Lide, CRC Handbook of Chemistry and Physics, 84th ed., CRC Press London, UK, (2003).

⁶G. C. He, R. M. Wei, X. L. Zhu, Y. L. Hua, X. Shao, P. W. Zhang, and C. Q. Xie, Appl. Surf. Sci. 488, 46 (2019).

⁷T. M. Tritt, Thermal Conductivity: Theory, Properties, and Applications, Springer, New York, USA, (2004).

⁸W. J. Zhang, Y. Liu, R. G. Cao, Z. H. Li, Y. H. Zhang, Y. Tang, and K. N. Fan, J. Am. Chem. Soc. 130, 15581 (2008).

⁹H. L. Gao, L. Xu, F. Long, Z. Pan, Y. X. Du, Y. Lu, J. Ge, and S. H. Yu, Chem. Int. Ed. 53, 4561 (2014).

¹⁰V. Novotny, P. P. M. Meincke, and J. H. P. Watson, Phys. Rev. Lett. 28, 901 (1972).