Supplementary Information

β-Ga_2O_3: a potential high temperature thermoelectric material

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Supplementary Figures

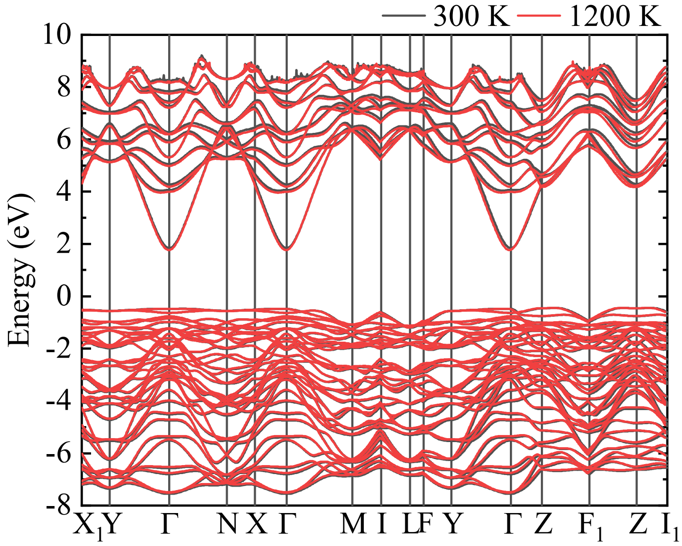

Fig. S1 The calculated energy band structure of β-Ga_2O_3 applied different temperature lattice parameters considering thermal expansion effects.

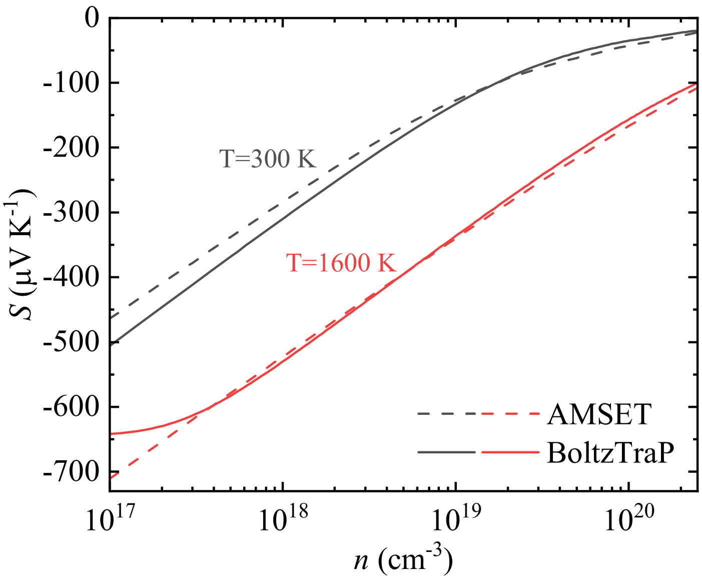

Fig. S2 The calculated Seebeck coefficient S of n-type β-Ga_2O_3 at 300 K and 1600 K applied different softwares (AMSET and BoltzTraP).

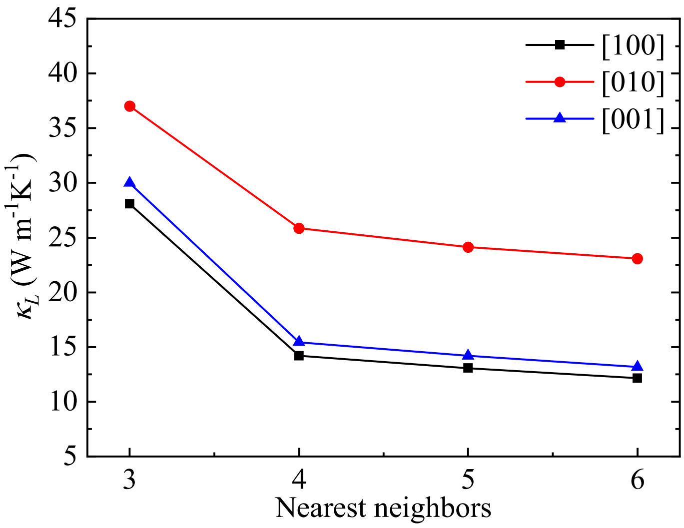

Fig. S3 The lattice thermal conductivity of β-Ga_2O_3 with respect to the nearest neighbors for the anharmonic inter-atomic force constants.

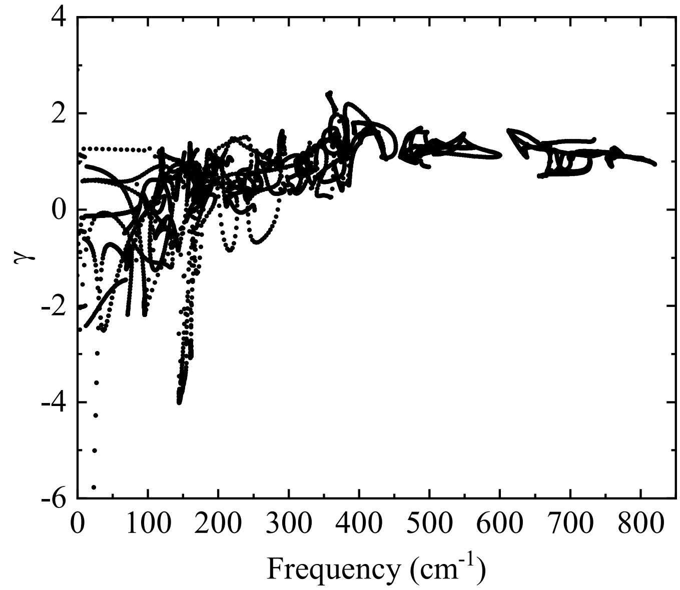

Fig. S4 The calculated mode Gruneisen parameters γ with respect to phonon frequency of β-Ga_2O_3 at 300 K.

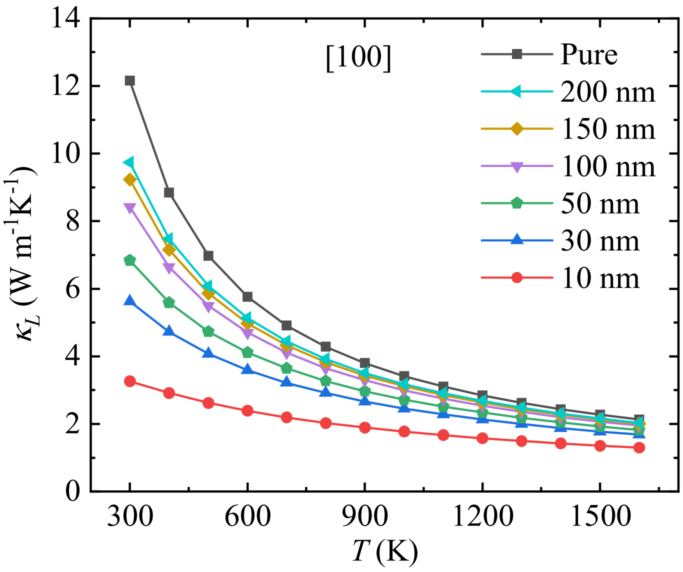

Fig. S5 The calculated lattice thermal conductivity of finite-size (10, 30, 50, 100, 150 and 200 nm) β-Ga_2O_3 as a function of temperature along [100] direction.

Supplementary Tables

Table S1 The calculated PO phonon frequency ω_{po} (THz), high-frequency ϵ_∞ and static ϵ_s dielectric constants of β-Ga_2O_3.

Parameter	ω_{po}	ϵ_∞	ϵ_s
Calculated Value	24.05	4.37	6.20

Table S2 The calculated elastic constants C_{ij} (GPa) of β-Ga_2O_3, compared with the previous data.

	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}
β-Ga_2O_3	363.07	474.61	459.25	154.97	90.10	130.28	172.52
	C_{13}	C_{23}	C_{16}	C_{26}	C_{36}	C_{45}	
β-Ga_2O_3	134.16	107.34	-9.90	20.76	1.03	18.90	

Supplementary Notes

Supplementary Notes 1. The elastic properties

The β-Ga_2O_3 compound has the base centered monoclinic structure, with 13 independent elastic constants (C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}, C_{12}, C_{13}, C_{23}, C_{16}, C_{26}, C_{36} and C_{45}).[1] The bulk modulus *B* and the shear modulus *G* can be given by

$$B_V = \frac{1}{9}[C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})] \tag{1}$$

$$G_V = \frac{1}{15}[C_{11} + C_{22} + C_{33} + 3(C_{44} + C_{55} + C_{66}) - (C_{12} + C_{13} + C_{23})] \tag{2}$$

$$B_R = \Omega[a(C_{11} + C_{22} - 2C_{13}) + b(2C_{13} - 2C_{11} - C_{23}) + c(C_{16} - 2C_{36}) + d(2C_{13} + 2C_{23} - C_{12} - 2C_{33}) + 2e(C_{36} - C_{16}) + f]^{-1} \tag{3}$$

$$G_R = 15\left\{\frac{4[a(C_{11}+C_{33}+C_{13})+b(C_{11}-C_{13}-C_{23})+c(C_{16}+C_{36})+d(C_{33}-C_{12}-C_{23}-C_{13})+e(C_{16}-C_{36})+f]}{\Omega} + 3\left[\frac{g}{\Omega} + (C_{44} + C_{55})/(C_{44}C_{55} - C_{45}^2)\right]\right\}^{-1} \tag{4}$$

Where,

$$a = C_{22}C_{66} - C_{26}^2$$

$$b = C_{23}C_{66} - C_{26}C_{36}$$

$$c = C_{12}C_{26} - C_{16}C_{22}$$

$$d = C_{12}C_{66} - C_{16}C_{26}$$

$$e = C_{12}C_{36} - C_{16}C_{23}$$

$$f = C_{11}(C_{33}C_{66} - C_{36}^2) - C_{13}(C_{13}C_{66} - C_{16}C_{36}) + C_{16}(C_{13}C_{36} - C_{16}C_{33}) + C_{36}(C_{23}C_{26} - C_{36}C_{22})$$

$$g = C_{11}C_{22}C_{33} - C_{11}C_{23}^2 - C_{22}C_{13}^2 - C_{33}C_{12}^2 + 2C_{12}C_{13}C_{23}$$

$$\Omega = 2[C_{16}C_{36}(C_{22}C_{13} - C_{12}C_{23}) + C_{16}C_{26}(C_{33}C_{12} - C_{13}C_{23}) + C_{26}C_{36}(C_{11}C_{23} - C_{12}C_{13})] - [C_{16}^2(C_{22}C_{33} - C_{23}^2) + C_{26}^2(C_{11}C_{33} - C_{13}^2) + C_{36}^2(C_{11}C_{22} - C_{12}^2)] + gC_{66}$$

In terms of the Voigt-Reuss-Hill approximations[2], *B* and *G* can be obtained by

$$B = \frac{1}{2}(B_V + B_R) \tag{5}$$

$$G = \frac{1}{2}(G_V + G_R) \tag{6}$$

The longitude (v_l) and shear (v_s) sound velocity can be written as

$$v_l = \sqrt{\frac{B+4/3G}{\rho}} \quad (7)$$

$$v_s = \sqrt{\frac{G}{\rho}} \quad (8)$$

The averaged sound velocity v_a is obtained by

$$v_a = \left[\frac{1}{3}\left(\frac{1}{v_l^3} + \frac{2}{v_s^3}\right)\right]^{-1/3} \quad (9)$$

The Gruneisen parameter γ is written by[3]

$$\gamma = \frac{3}{2}\left(\frac{1+v_p}{2-3v_p}\right) \quad (10)$$

Where, $v_p = \frac{1-2(v_s/v_l)^2}{2-2(v_s/v_l)^2}$.

The Debye temperature Θ_D can be given by[3]

$$\Theta_D = \frac{h}{k_B}\left[\frac{3N}{4\pi V}\right]^{1/3} v_a \quad (13)$$

Where, ρ is the density, *h* is Planck's constant, k_B is the Boltzmann constant, *N* is the number of atoms in the unit cell, *V* is the unit cell volume. According to the above formula, the elastic properties of *β*-Ga_2O_3 is obtained.

Supplementary References

1. Z. J. Wu, E. J. Zhao, H. P. Xiang, X. F. Hao, X. J. Liu and J. Meng, *Physical Review B*, 2007, **76**, 054115.
2. R. Hill, *Proceedings of the Physical Society*, 1952, **65**, 349-354.
3. Y. Xiao, C. Chang, Y. L. Pei, D. Wu, K. L. Peng, X. Y. Zhou, S. K. Gong, J. Q. He, Y. S. Zhang, Z. Zeng and L. D. Zhao, *Physical Review B*, 2016, **94**, 125203.