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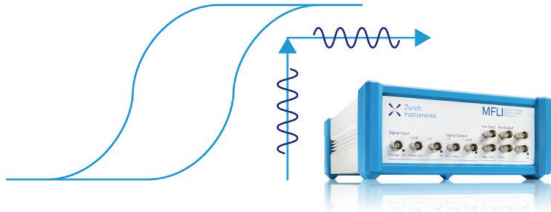
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**Note:** This paper is part of the Special Topic on Ultrawide Bandgap Semiconductors.

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## ABSTRACT

Power electronics seek to improve power conversion of devices by utilizing materials with a wide bandgap, high carrier mobility, and high thermal conductivity. Due to its wide bandgap of 4.5 eV,  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> has received much attention for high-voltage electronic device research. However, it suffers from inefficient thermal conduction that originates from its low-symmetry crystal structure. Rutile germanium oxide (r-GeO<sub>2</sub>) has been identified as an alternative ultra-wide-bandgap (4.68 eV) semiconductor with a predicted high electron mobility and ambipolar dopability; however, its thermal conductivity is unknown. Here, we characterize the thermal conductivity of r-GeO<sub>2</sub> as a function of temperature by first-principles calculations, experimental synthesis, and thermal characterization. The calculations predict an anisotropic phonon-limited thermal conductivity for r-GeO<sub>2</sub> of 37 W m<sup>-1</sup> K<sup>-1</sup> along the *a* direction and 58 W m<sup>-1</sup> K<sup>-1</sup> along the *c* direction at 300 K where the phonon-limited thermal conductivity predominantly occurs via the acoustic modes. Experimentally, we measured a value of 51 W m<sup>-1</sup> K<sup>-1</sup> at 300 K for hot-pressed, polycrystalline r-GeO<sub>2</sub> pellets. The measured value is close to our directionally averaged theoretical value, and the temperature dependence of  $\sim 1/T$  is also consistent with our theory prediction, indicating that thermal transport in our r-GeO<sub>2</sub> samples at room temperature and above is governed by phonon scattering. Our results reveal that high-symmetry UWBG materials, such as r-GeO<sub>2</sub>, may be the key to efficient power electronics.

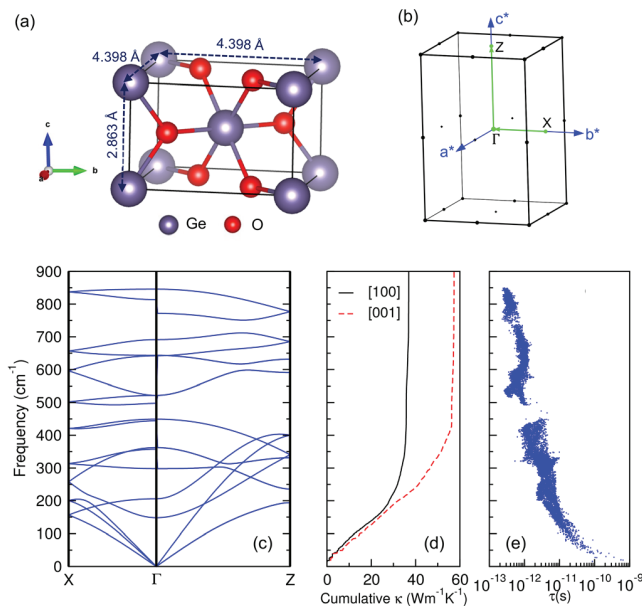
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As the critical dielectric breakdown field of materials increases non-linearly with the increasing bandgap, ultra-wide bandgap (UWBG) semiconductors with gaps wider than GaN (3.4 eV) have emerged as compelling materials for high-power electronic applications.<sup>1</sup> In addition to their wide bandgap, other desirable material properties for power electronics include the possibility of both *n*-type and *p*-type doping, high carrier mobilities to reduce energy lost during device operation, and high thermal conductivity to efficiently remove the generated waste heat.

Numerous UWBG semiconductors have been explored for power electronics; however, many of them face significant challenges in efficient thermal management. For example,  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> is one of the most popular UWBG materials, but its poor intrinsic thermal conductivity  $\kappa$  (11 W m<sup>-1</sup> K<sup>-1</sup> and 27 W m<sup>-1</sup> K<sup>-1</sup> along the  $\vec{a}$  and  $\vec{b}$  directions, respectively)<sup>2,3</sup> is a crucial drawback. Other state-of-the-art UWBG materials, such as AlGaN/AlN and diamond, exhibit high intrinsic thermal conductivities. However, AlGaN/AlN is typically grown epitaxially on sapphire substrates with low thermal conductivity (34.6 W m<sup>-1</sup> K<sup>-1</sup>), whereas the high cost of single-crystal AlN and diamond substrates that conduct heat efficiently poses an obstacle for adoption in devices.

Recently, first-principles calculations identified rutile GeO<sub>2</sub> (r-GeO<sub>2</sub>) as a promising but unexplored UWBG material for applications in high-power electronics. Its ultra-wide bandgap, experimentally measured at 4.68 eV<sup>4</sup> and theoretically evaluated at 4.44–4.68 eV,<sup>5,6</sup> is similar to that of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>. Moreover, whereas  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> can only be doped *n*-type, r-GeO<sub>2</sub> has promising doping properties with shallow ionization energies for donors and an ionization energy of 0.45 eV for Al acceptors.<sup>6</sup> In addition, we recently evaluated its intrinsic phonon-limited electron mobility and dielectric breakdown and predicted its Baliga Figure of Merit (BFOM) to be higher than that of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>.<sup>7</sup> Unlike the monoclinic crystal structure of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, r-GeO<sub>2</sub> has a more symmetric tetragonal crystal structure with fewer atoms in the unit cell [Fig. 1(a)]. Thus, we expect that the intrinsic phonon-limited thermal conductivity of r-GeO<sub>2</sub> is higher than that of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> due to reduced phonon-band folding. Moreover, we anticipate that r-GeO<sub>2</sub> can be grown on thermally conductive rutile substrates such as SnO<sub>2</sub> ( $\kappa \sim 100$  W m<sup>-1</sup> K<sup>-1</sup>).<sup>8</sup> However, the thermal conductivity of r-GeO<sub>2</sub> has not previously been reported.

In this work, we investigate the thermal conductivity of r-GeO<sub>2</sub> by both first-principles calculations and experimental measurements on polycrystalline samples. Our calculations show that the intrinsic



**FIG. 1.** (a) and (b) (a) Atomic structure and (b) Brillouin zone of rutile  $\text{GeO}_2$  (c) phonon dispersion of  $\text{r-GeO}_2$ , including polar LO-TO splitting; (d) cumulative thermal conductivity at 300 K along the  $\perp \vec{c}$  and  $\parallel \vec{c}$  directions. The bulk thermal conductivity at 300 K is  $37 \text{ W m}^{-1} \text{ K}^{-1} \perp \vec{c}$  and  $58 \text{ W m}^{-1} \text{ K}^{-1} \parallel \vec{c}$ . The acoustic modes have the largest contribution to thermal conductivity along both crystallographic directions. (e) Phonon lifetime due to three-phonon scattering as a function of phonon frequency. The lifetimes are the longest for the acoustic modes and show an overall decrease with increasing phonon frequency.

phonon-limited thermal conductivity is anisotropic, with values of  $37 \text{ W m}^{-1} \text{ K}^{-1} \perp \vec{c}$  and  $58 \text{ W m}^{-1} \text{ K}^{-1} \parallel \vec{c}$  at 300 K, reflecting the anisotropy of the rutile crystal structure. We find a directionally averaged thermal conductivity at 300 K of  $44 \text{ W m}^{-1} \text{ K}^{-1}$  (theory) and  $51 \text{ W m}^{-1} \text{ K}^{-1}$  (experiment), indicating that  $\text{r-GeO}_2$  is a superior thermal conductor to  $\beta\text{-Ga}_2\text{O}_3$  ( $11 \text{ W m}^{-1} \text{ K}^{-1} \parallel \vec{a}$  and  $27 \text{ W m}^{-1} \text{ K}^{-1} \parallel \vec{b}$ ) and can overcome the thermal-dissipation limitations of  $\beta\text{-Ga}_2\text{O}_3$ -based devices.

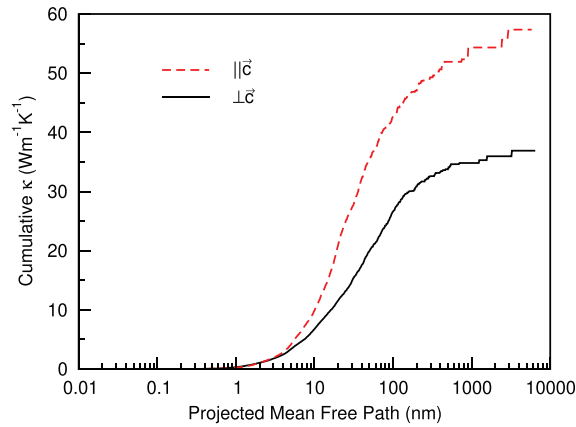
Our calculations are based on the Boltzmann transport equation (BTE) as implemented in the almaBTE software.<sup>9</sup> The second-order (harmonic) interatomic force constants (IFCs) and Born effective charges were calculated within Quantum ESPRESSO<sup>10</sup> using density functional theory (DFT) and density functional perturbation theory under the local-density approximation (LDA).<sup>11,12</sup> To obtain accurate phonon frequencies, a  $\text{Ge}^{4+}$  pseudopotential with the  $3d$  electrons in the valence was used. The plane wave cutoff energy of 140 Ry converges the total energy of the system to within 1 mRy/atom. We generated the crystal structure of  $\text{r-GeO}_2$  starting from the experimental lattice parameters (space group =  $\text{P4}_2/\text{mmn}$ , Ge site = 0, 0, 0 and O site = 0.3060, 0.3060, 0).<sup>13</sup> The structure was relaxed until the total pressure in the unit cell was 0.01 kbar and forces on the atoms were less than  $|5 \times 10^{-6}| \text{ Ry/a}_0$ . The relaxed parameters  $a = 4.3736 \text{ Å}$  and  $c = 2.8674 \text{ Å}$  differ from experiment ( $a = 4.4066 \text{ Å}$  and  $c = 2.8619 \text{ Å}$ )<sup>13</sup> by only 0.7% and 0.2%, respectively. The phonon frequencies were calculated on a  $6 \times 6 \times 9$  Brillouin zone (BZ) [Fig. 1(b)] sampling grid, thus producing second-order IFCs on the same

supercell size. The third-order (anharmonic) IFCs were calculated using finite displacements on a  $4 \times 4 \times 4$  supercell by manually shifting selected atoms and calculating the produced forces on surrounding atoms. A 0.5 nm nearest-neighbor distance cutoff was applied. The calculated relaxed structure, IFCs, and Born effective charges were applied within the almaBTE software, where an  $18 \times 18 \times 27$  BZ sampling grid was used to calculate the thermal conductivity of  $\text{r-GeO}_2$  with the full BTE.

To synthesize bulk pellets of rutile- $\text{GeO}_2$ , quartz-phase  $\text{GeO}_2$  powders (Alfa Aesar, 99.999%) were loaded into a 10 mm-diameter graphite die and hot pressed at  $800^\circ\text{C}$  under a pressure of 100 MPa for 3 h. The heating and cooling rate was  $220^\circ\text{C/h}$ , and the pressing chamber was kept under vacuum ( $10^{-2}$  Torr) throughout the process. X-ray diffraction (Rigaku Smartlab diffractometer equipped with a  $1.54 \text{ Å}$  Cu K  $\alpha$  source) and scanning electron microscopy (JEOL IT500 SEM) were used to characterize the crystal structure and microstructure of our samples. The specific heat capacity and thermal diffusivity of  $\text{r-GeO}_2$  pellets were measured on a laser flash system (Linseis LFA-1000) from room temperature to 677 K. Pellets were lightly coated with graphite spray, and the measurement was performed under flowing  $\text{N}_2$  gas. For each measurement step, we measured a Pyroceram 9606 reference sample and determined the measurement error, which is  $< 1\%$  for specific heat capacity and  $< 4\%$  for thermal diffusivity. The mass density was measured using Helium gas pycnometry on a Micromeritics Accucyc II 1340.

The calculated phonon dispersion of  $\text{r-GeO}_2$  is shown in Fig. 1(c). Longitudinal optical-transverse optical (LO-TO) splitting at  $\Gamma$  is observed for the four infrared (IR) active modes, with three of the modes splitting along the  $\Gamma$ -X direction and one along  $\Gamma$ -Z. The Born effective charges are +4.45 for Ge and -2.23 for O. The sound velocities of  $\text{r-GeO}_2$  were reported previously (4.67–9.44 km/s)<sup>7</sup> and are higher than those of both GaN (3.69–7.67 km/s) and  $\beta\text{-Ga}_2\text{O}_3$  (2.90–7.55 km/s).<sup>14,15</sup> The LA modes along the  $\Gamma$ -Z direction extend up to a frequency of  $400 \text{ cm}^{-1}$  that is approximately twice as large as that along  $\Gamma$ -X ( $205 \text{ cm}^{-1}$ ). This is due to the combination of a 1.4 higher LA sound velocity along  $\Gamma$ -Z (9.44 km/s) than along  $\Gamma$ -X (6.74 km/s)<sup>7</sup> and the 1.5 times larger dimensions of the first BZ of  $\text{r-GeO}_2$  along  $\Gamma$ -Z. At the edge of the BZ along  $\Gamma$ -Z, the frequency of the longitudinal-acoustic (LA) mode surpasses those of six optical modes, which indicates that simultaneous thermal activation of acoustic and optical modes can occur.

Figure 1(d) shows the thermal conductivity at 300 K and its cumulative distribution as a function of phonon frequency. The thermal conductivity at 300 K is  $37 \text{ W m}^{-1} \text{ K}^{-1} \perp \vec{c}$  and  $58 \text{ W m}^{-1} \text{ K}^{-1} \parallel \vec{c}$ , resulting in a directional average of  $44 \text{ W m}^{-1} \text{ K}^{-1}$ . While several optical modes are mixed with the acoustic modes near the zone edges, a significant portion of the cumulative thermal conductivity is reached at the maximum acoustic-phonon frequencies. Along the  $\perp \vec{c}$  direction, 77% of the total thermal conductivity is reached at the frequency of  $205 \text{ cm}^{-1}$ . The percentage is even higher for the  $\parallel \vec{c}$  direction, with 95% of the total thermal conductivity reached at  $400 \text{ cm}^{-1}$ . Therefore, acoustic modes are the primary phonon modes responsible for heat conduction in  $\text{r-GeO}_2$ . Since the characteristic frequencies for the saturation of the cumulative thermal-conductivity distribution coincide with the highest LA mode frequencies along the two main crystallographic directions, we conclude that the LA modes are likely the dominant modes that contribute to the thermal conductivity. Moreover, the ratio of the

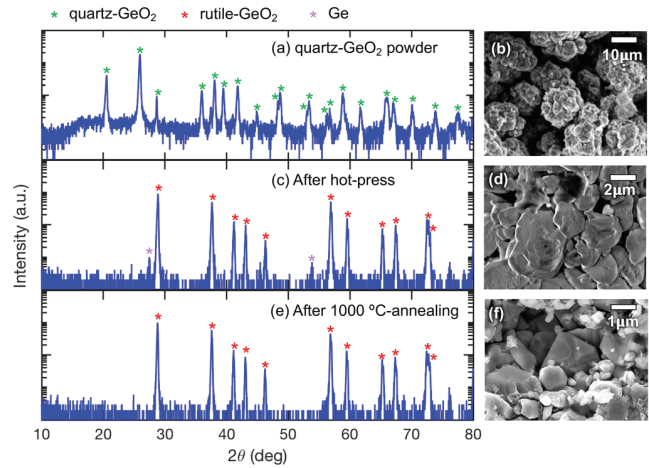


**FIG. 2.** Cumulative thermal-conductivity distribution of r-GeO<sub>2</sub> at 300 K as a function of the phonon mean free path. 90% of the maximum thermal conductivity along both directions is reached for a mean free path of 0.4  $\mu\text{m}$ .

thermal conductivity along the two axes ( $\kappa_{||c}/\kappa_{\perp c} = 1.54$ ) is similar to the ratio of the corresponding LA sound velocities ( $v_{\text{LA},||c}/v_{\text{LA},\perp c} = 1.4$ ), further indicating that the LA modes dominate thermal transport in r-GeO<sub>2</sub>. The phonon lifetimes due to three-phonon scattering are plotted as a function of phonon frequency in Fig. 1(e). The lifetimes are the longest for the acoustic modes and show an overall decrease with increasing phonon frequency.

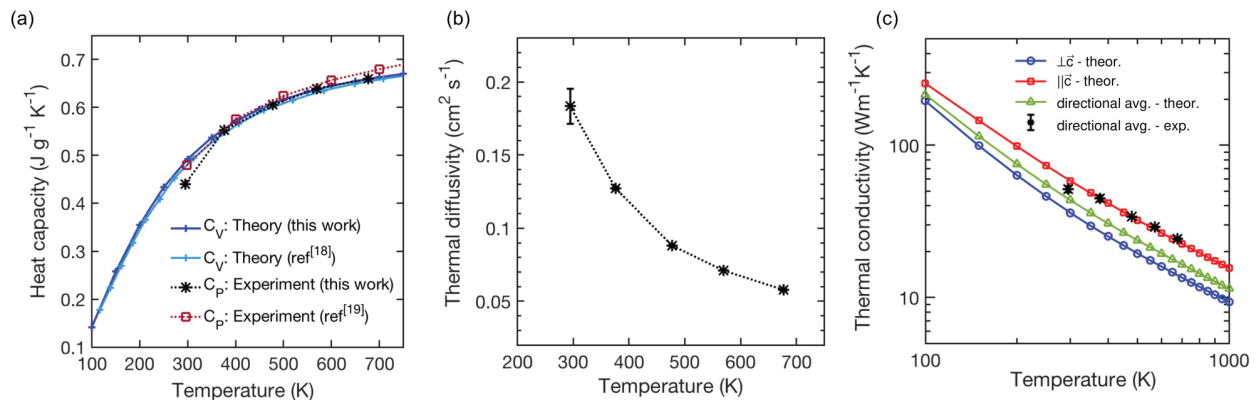
The dependence of  $\kappa$  on the phonon mean free path (MFP) proves to be useful to understand the thermal conductivity of polycrystalline samples and thin films, for which the MFP is determined by the grain size and film thickness, respectively. Figure 2 shows the cumulative thermal-conductivity distribution at 300 K along the  $\perp c$  and  $\parallel c$  directions as a function of phonon MFP. Along both directions, 90% of the maximum  $\kappa$  is reached at a phonon MFP of 0.4  $\mu\text{m}$ .

Figure 3 shows the x-ray diffraction (XRD) pattern and scanning electron microscopy (SEM) images for (a) and (b) quartz-GeO<sub>2</sub>



**FIG. 3.** X-ray diffraction pattern and scanning electron microscope images of (a) and (b) GeO<sub>2</sub> powder, (c) and (d) a GeO<sub>2</sub> pellet after hot pressing at 800 °C and 100 MPa, and (e) and (f) a GeO<sub>2</sub> pellet after hot pressing (800 °C, 100 MPa) and subsequent annealing (1000 °C, air). A phase-pure rutile GeO<sub>2</sub> pellet is obtained through hot-pressing and subsequent annealing, with grain sizes of  $1.50 \pm 0.30 \mu\text{m}$ .

powder and (c) and (d) the initial hot-pressed pellet, showing nearly 100% phase conversion to r-GeO<sub>2</sub> after hot-press. However, we observe < 2% impurity Ge phase after hot pressing. In order to oxidize the Ge impurity phase, we annealed the hot-pressed pellet at 1000 °C in air [Figs. 3(e) and 3(f)]. Our XRD analysis shows that the final product is a single-phase, polycrystalline rutile GeO<sub>2</sub> pellet with a grain size of  $1.50 \pm 0.30 \mu\text{m}$ . We, therefore, conclude that the measured thermal conductivity of our polycrystalline sample is close to the intrinsic phonon-limited bulk value. We also measured a mass-density ( $\rho$ ) value of  $6.39 \pm 0.04 \text{ g/cm}^3$  for the final product, which is 1.9% higher than the ideal value for rutile GeO<sub>2</sub> ( $6.27 \text{ g/cm}^3$ ).



**FIG. 4.** (a) The calculated constant-volume specific heat ( $C_V$ ) of r-GeO<sub>2</sub> and the measured constant-pressure specific heat ( $C_P$ ) of r-GeO<sub>2</sub> as a function of temperature are in good agreement with each other and with previous work.<sup>18,19</sup> (b) Thermal diffusivity of polycrystalline r-GeO<sub>2</sub> measured as a function of temperature by the laser-flash method. (c) Experimental and theoretical thermal conductivity of r-GeO<sub>2</sub> from 100 K to 1000 K on the logarithmic scale. The theoretical values were calculated along both crystallographic directions and averaged according to  $\kappa_{\text{avg}} = \frac{2}{3}\kappa_a + \frac{1}{3}\kappa_c$ . Experimental measurements were performed on a polycrystalline r-GeO<sub>2</sub> sample with an average grain size of  $1.50 \pm 0.30 \mu\text{m}$ . The measured values are slightly higher than the directionally averaged theoretical values, but a consistent temperature dependency trend is observed between the theoretical and the experimental results.



Figures 4(a) and 4(b) show the specific heat capacity ( $C_p$ ) and the thermal diffusivity ( $\alpha$ ) of r-GeO<sub>2</sub> as a function of temperature. The experimental constant-pressure specific heat is in good agreement with the calculated constant-volume specific heat capacity ( $C_V$ ) since the difference between the two quantities  $C_p - C_V = \frac{T \cdot V \cdot \alpha^2}{K}$  is estimated to be less than 1% at room temperature, where  $V$  is the molar volume ( $1.597 \times 10^{-7} \text{ m}^3/\text{g}$ ),  $\alpha$  is the thermal-expansion coefficient ( $14.2 \times 10^{-6} \text{ K}^{-1}$ ), and  $K$  is the compressibility ( $4.05 \times 10^{-12} \text{ Pa}^{-1}$ ).<sup>16,17</sup> The thermal conductivity ( $\kappa = \alpha \cdot C_p \cdot \rho$ ) is plotted as a function of temperature in Fig. 4(c) and compared with our calculated results. We observed that the measured thermal conductivity is slightly higher than the directionally averaged calculated values. We also observed the temperature dependence of the measured thermal conductivity to be consistent with the trend predicted by theory.

The thermal conductivity is one of the most important criteria to determine the performance of UWBG materials in power applications.  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> is one of the most promising materials for devices due to the high breakdown field; however, it suffers from poor thermal conduction due to the low symmetry of the monoclinic crystal structure. Our results demonstrate r-GeO<sub>2</sub> as an alternative UWBG material with superior thermal properties. The measured thermal conductivity of r-GeO<sub>2</sub> at 300 K ( $51 \text{ W m}^{-1} \text{ K}^{-1}$ ) is approximately 2 times higher than the highest value of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>.<sup>2</sup> Also, while  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> can only be grown on thermally poor substrates (e.g., Al<sub>2</sub>O<sub>3</sub>), the higher symmetry of r-GeO<sub>2</sub> may enable electronic device architectures with better thermal conduction. The higher thermal conductivity of r-GeO<sub>2</sub>, along with its predicted ambipolar dopability and higher BFOM compared to  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, accentuates its potential for UWBG electronic applications.

In conclusion, we report the results of first-principles calculations and experimental measurements for the thermal conductivity of r-GeO<sub>2</sub> as a function of temperature. Our calculations predict phonon-limited thermal conductivities of  $37 \text{ W m}^{-1} \text{ K}^{-1} \perp \vec{c}$  and  $58 \text{ W m}^{-1} \text{ K}^{-1} \parallel \vec{c}$  at 300 K. The measured thermal conductivity of our synthesized polycrystalline r-GeO<sub>2</sub> pellets with grain sizes of  $1.50 \pm 0.30 \mu\text{m}$  at room temperature is  $51 \text{ W m}^{-1} \text{ K}^{-1}$ . From theory, we show that thermal transport occurs primarily through phonons with mean free paths shorter than  $0.4 \mu\text{m}$ , indicating that our experimental measurements are in the range of the single-crystal values. Our theoretical and experimental thermal conductivity results showcase that r-GeO<sub>2</sub> is a promising UWBG material with superior thermal conductivity to  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> for efficient heat management in power-electronics applications.

## AUTHORS' CONTRIBUTIONS

S.C. and K.A.M. contributed equally to this work.

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## DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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