High thermal conductivity in wafer-scale cubic silicon carbide crystals

High thermal conductivity electronic materials are critical components for high-performance electronic and photonic devices as both active functional materials and thermal management materials. We report an isotropic high thermal conductivity exceeding 500 W m⁻¹K⁻¹ at room temperature in high-quality wafer-scale cubic silicon carbide (3C-SiC) crystals, which is the second highest among large crystals (only surpassed by diamond). Furthermore, the corresponding 3C-SiC thin films are found to have record-high in-plane and cross-plane thermal conductivity, even higher than diamond thin films with equivalent thicknesses. Our results resolve a long-standing puzzle that the literature values of thermal conductivity for 3C-SiC are lower than the structurally more complex 6H-SiC. We show that the observed high thermal conductivity in this work arises from the high purity and high crystal quality of 3C-SiC crystals which avoids the exceptionally strong defect-phonon scatterings. Moreover, 3C-SiC is a SiC polytype which can be epitaxially grown on Si. We show that the measured 3C-SiC-Si thermal boundary conductance is among the highest for semiconductor interfaces. These findings provide insights for fundamental phonon transport mechanisms, and suggest that 3C-SiC is an excellent wide-bandgap semiconductor for applications of next-generation power electronics as both active components and substrates.

Silicon carbide (SiC) plays a fundamental role in many emerging technologies such as power electronics, optoelectronics, and quantum computing². SiC based power devices can lead a revolution in power electronics to replace Si-based technology due to its fast switching speeds, low losses, and high blocking voltage. In power electronics and optoelectronics, the high localized heat flux leads to overheating of devices. The increased device temperature degrades their performance and reliability, making thermal management a grand challenge. High thermal conductivity (κ) is critical in thermal management design of these electronics and optoelectronics, especially for high-power devices.

Current high κ electronic materials such as hexagonal SiC and AlN have room-temperature c-axis κ of ~320 W m⁻¹K⁻¹ for 6H-SiC, ~350 W m⁻¹K⁻¹ for 4H-SiC, and ~320 W m⁻¹K⁻¹ for AlN, which are lower than metals such as silver and copper (~430 and 400 W m⁻¹K⁻¹)¹,². The widely used high κ value (490 W m⁻¹K⁻¹) for 6H-SiC is from Slack’s...
measurements back to 1964 with a thermocouple-based steady-state technique. Recent more advanced measurements based on time-domain thermoreflectance (TDTR) reduced the errors and corrected this value to ~320 W m⁻¹ K⁻¹ for 6H-SiC, which is consistent with first-principles calculations of perfect single crystal 6H-SiC based on density functional theory (DFT). The excellent agreement of the measured 6H-SiC thermal conductivity with the predicted intrinsic thermal conductivity shows the high quality of current commercially available 6H-SiC.

Compared with the extensively studied and widely used hexagonal phase SiC polytypes (6H and 4H), the cubic phase SiC (3C) is much less well understood even though it potentially has the best electronic properties and much higher κ. The metal oxide semiconductor field effect transistor (MOSFET) based on 3C-SiC has the highest channel mobility ever presented on any SiC polytype, which produces a large reduction in the power consumption of power switching devices. 3C-SiC is a SiC polytype which can be grown on Si. A long-standing puzzle about the measured κ of 3C-SiC is that the literature value is lower than that of the structurally more complex 6H phase and much lower than the theoretically predicted intrinsic thermal conductivity of 3C-SiC. This contradicts the prediction of simple theory that the structural complexity and κ are inversely correlated. To explain the anomalously low κ of 3C-SiC in the literature, A. Katre et al. studied all the measured thermal conductivity and impurity of 3C-SiC in the literature and attributed the low κ to exceptionally strong boron defect-phonon scattering, which is even stronger than phonon scattering by vacancies. 0.1% boron creates a factor of 2 decrease in κ while the same reduction is created by 2% substitutional nitrogen. However, experimental validation is still lacking partly due to the challenges in growing high-quality 3C-SiC crystals. The material growth techniques and successful quality control of 6H-SiC crystals laid the foundation for current wide adoption of 6H-SiC electronics while the applications of 3C-SiC electronics are limited by the crystal quality and purity.

The potential high κ of 3C-SiC not only facilitates applications which use 3C-SiC as active electronic materials, but also enables 3C-SiC to be a thermal management material which cools devices made of other semiconductors. For thermal management materials, diamond has the highest isotropic κ among all bulk materials but is limited by its high cost, small wafer size, and difficulty in heterogeneous integration with other semiconductors. For thermal management applications with high thermal boundary conductance (TBC), it is observed that carbon-based nanomaterials such as graphene and carbon nanotubes decrease significantly when assembling together or with other materials. Recently, great progress has been achieved in the discovery of isotropic high κ in high-purity boron-based crystals, such as cubic BN and natural and isotope-enriched cubic BN, and natural and isotope-enriched cubic BP, but all the crystal sizes are millimeter-scale or smaller. The technical difficulties in growth of high-purity large crystals prevent these high κ thermal management materials from scalable manufacturing that is required for the processing of devices. Further heterogeneous integration of these high κ thermal management materials with other semiconductors with high TBC is also challenging.

Here, we report an isotropic high κ exceeding 500 W m⁻¹ K⁻¹ at room temperature in a high-purity wafer-scale free-standing 3C-SiC bulk crystal grown by low-temperature chemical vapor deposition. The measured κ agrees well with the first-principles predicted intrinsic κ of perfect single-crystal 3C-SiC. Moreover, 3C-SiC can be heterogeneously integrated with Si and AlN by epitaxial growth. The in-plane and cross-plane κ of corresponding 3C-SiC thin films are measured by beam-offset time-domain thermoreflectance (BO-TDTR). Further structural analysis such as Raman spectroscopy, X-ray diffraction (XRD), high-resolution scanning transmission electron microscopy (HR-STEM), electron backscatter diffraction (EBSD), and second ion mass spectroscopy (SIMS) are performed to understand the relationship between microstructure, composition, and thermal conductivity. Additionally, the TBC of 3C-SiC epitaxial interfaces with Si and AlN are studied by TDTR.

**Results**

3C-SiC has a less complex crystal structure than 6H-SiC (Fig. 1a). Therefore, higher κ than 6H phase is predicted for 3C-SiC single crystal. We obtain a free-standing 3C-SiC wafer (Fig. 1b) by growing 3C-SiC on a silicon substrate and then etching away the Si substrate. More details about samples can be found in Methods section. The wafer has a yellow color because of two reasons. First, the bandgap of 3C-SiC is 2.3 eV which corresponds to the energy of photons with wavelength of 539 nm. The intrinsic absorption of 3C-SiC makes it look yellow. Second, the nitrogen defects in the 3C-SiC crystal also possibly contribute to the yellow color. Peaks (795 cm⁻¹ for TO and 969 cm⁻¹ for LO) in Raman spectrum measured on the 3C-SiC crystal (Fig. 1c) agree well with the Raman peaks of 3C-SiC in the literature (796 cm⁻¹ for TO and 970 cm⁻¹ for LO). Fig. 1d shows rocking curve of the X-ray diffraction of the 3C-SiC crystal. The full width at half maximum (FWHM) of the (111) peak is 158 arcsec, showing the high crystal quality of the 3C-SiC crystal. To further probe the crystal structure of the 3C-SiC, we obtained an annular dark field STEM image (Fig. 1e) with atomically resolved lattices. The Fast Fourier transform (FFT) of the STEM image is shown in the inset of Fig. 1e. Figure 1f shows the selected area electron diffraction (SAED) pattern in a STEM, further confirming the SiC crystal is the cubic phase. More details about Raman measurements, STEM, and SAED can be found in Methods section.

We performed TDTR measurements on the freestanding bulk 3C-SiC to determine the crystal orientation. The EBSD data of both the face close to Si substrate and the growth face shows single (111) orientation over the entire scanned area (2.4 mm x 0.8 mm). More details can be found in the Methods section and SI. To figure out the main impurity concentrations in 3C-SiC, SIMS was used to measure the concentrations of boron, nitrogen, and oxygen impurities. The oxygen and nitrogen concentrations measured from the growth surface are 6.6 × 10¹⁶ atoms cm⁻² and 5.5 × 10¹⁵ atoms cm⁻², respectively. The oxygen and nitrogen concentrations measured from the face adjacent to the Si substrate before etching away Si are 2.3 × 10¹⁵ atoms cm⁻² and 1.4 × 10¹⁵ atoms cm⁻², respectively. The concentrations of boron impurity are below the detection limit (~3 × 10¹⁰ atoms cm⁻³) for SIMS measurements on both faces. The measured low concentrations of impurities further confirm the high quality of the 3C-SiC crystals in this work and high κ is expected. The other point defects such as vacancies were not characterized due to technical difficulties but we expect low concentrations of them.

We performed TDTR measurements on the free-standing 3C-SiC bulk crystal from the growth face to obtain its thermal conductivity. Figure 2a shows an example of the TDTR ratio data (circles) and model fitting (solid line) for the bulk 3C-SiC sample with 5× objective and 9.3 MHz modulation frequency. The dash lines are model curves using κ 10% larger or 10% smaller than the best-fit κ to illustrate the measurement sensitivity. More details about the TDTR measurements can be found in the Methods section and SI. To evaluate the effect of ballistic thermal transport on TDTR measurements of high κ samples, we did multiple TDTR measurements with different spot sizes (10.7 μm for 5× objective, 5.5 μm for 10× objective, and 2.7 μm for 20× objective) and different modulation frequencies (1.9–9.3 MHz). We observed weak dependence of measured κ on the modulation frequency (Fig. 2b) while strong reduction in the measured κ for 20× compared to 5× and 10× (Fig. 2b). This reduction is due to the ballistic thermal transport in the sample and the mismatch in the distributions of phonons that carry heat across the metal transducer-sample interface.
and in the sample. We used 9.3 MHz and 5× objective for the remainder of the measurements on the \( \kappa \) of bulk 3C-SiC (Figs. 2c, 3). The thickness of the free-standing 3C-SiC bulk crystal (100 \( \mu \)m) is much larger than the dominant phonon mean free paths in 3C-SiC and the thermal penetration depth in the TDTR measurements (the phonon dispersion relation and phonon mean free path accumulated thermal conductivity of perfect 3C-SiC single crystal calculated by DFT are included in the SI).

The measured \( \kappa \) of 3C-SiC at room temperature is compared with other high \( \kappa \) crystals as a function of wafer size (Fig. 2c)\(^{11,12,13,20,22,23,26}\). The recently reported boron-based crystals have high \( \kappa \) but the achievable crystal sizes are millimeter-scale or smaller. Single crystal diamond has a larger wafer size, up to 2 inch, but wide-range adoptions are limited by the high cost and difficulty in heterogeneous integration with other semiconductors\(^{19,20,29}\). Heterogeneous epitaxial growth of single crystal diamond on Si and GaN is challenging\(^{29}\). Current chemical vapor deposited (CVD) polycrystalline diamond results in significantly reduced and anisotropic \( \kappa \)\(^{32,33}\).

The 3C-SiC wafer reported in this work can reach up to 6-inch in size with an isotropic high \( \kappa \) exceeding 500 W m\(^{-1}\)K\(^{-1}\). The measured \( \kappa \) of 3C-SiC is higher than all metals and the second highest among all large crystals (only surpassed by single crystal diamond). The \( \kappa \) of 3C-SiC at room temperature is ~50% higher than the c-axis \( \kappa \) of 6H-SiC and AlN, and ~40% higher than the c-axis \( \kappa \) of 4H-SiC.

We further measured the \( \kappa \) of bulk 3C-SiC crystal at high temperatures. The measured temperature dependent \( \kappa \) of bulk 3C-SiC is compared with previously measured \( \kappa \) values in the literature, \( \kappa \) values of perfect single crystal predicted by DFT, and that of other high \( \kappa \) crystals (See Fig. 3a, b). The measured \( \kappa \) agrees well with DFT-calculated \( \kappa \) of perfect single crystal 3C-SiC at all measured temperatures. The measured \( \kappa \) in this work is >50% higher than the literature values of 3C-SiC at room temperature, and surpasses that of the structurally more complex 6H-SiC. These results are consistent with the theoretical calculations that structural complexity and \( \kappa \) are inversely related\(^{17}\). The measured high \( \kappa \) resolves a long-standing puzzle about the abnormally low \( \kappa \) values in the literature which was attributed to the extrinsic defect-phonon scatterings in 3C-SiC\(^1\). Boron defects in 3C-SiC cause exceptionally strong phonon scatterings which results from the resonant phonon scattering by the boron impurity\(^1\). The measured boron impurity concentration is negligible (below the detection limit: 3 × 10\(^{13}\) atoms cm\(^{-3}\)) in our 3C-SiC crystals according to the SIMS measurements. The oxygen and nitrogen concentrations are also low (6.6 × 10\(^{17}\) atoms cm\(^{-3}\) and 5.8 × 10\(^{15}\) atoms cm\(^{-3}\)).

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We also compare the measured temperature dependent \( \kappa \) of bulk 3C-SiC crystals with that of AlN, 6H-SiC, and GaN. We include both the in-plane \( \kappa \) and cross-plane \( \kappa \) of 6H-SiC since the \( \kappa \) of 6H-SiC is anisotropic. The DFT-calculated \( \kappa \) values of perfect single crystals agree well with the measured \( \kappa \) values and both are proportional to the inverse of temperature due to the dominant phonon-phonon scatterings in these crystals at high temperatures. The measured \( \kappa \) values of 3C-SiC are 2.5 times as high as that of GaN, making 3C-SiC a potential candidate as substrates of GaN-based power electronics. The high \( \kappa \) of 3C-SiC will motivate the study of power electronics which use 3C-SiC as active
device material as a more advanced addition to currently wide-adopted 4H-SiC and 6H-SiC.

We performed beam-offset time-domain thermoreflectance (BO-
TDTR) on 3C-SiC thin films grown on Si substrates to obtain the in-
plane \( \kappa \) of 3C-SiC films\(^{24,31}\). During BO-TDTR measurements, the pump
beam is offset relative to the probe beam, as shown in Fig. 4a. An
example of the out-of-phase TDTR signal on a 2.52-\( \mu \)m-thick SiC film on
Si sample is shown as a function of the beam offset distance. The full
width at half maximum (FWHM) is a measure of the lateral heat
spreading which is used to fit for the in-plane \( \kappa \) of the 3C-SiC thin film. More
details about the BO-TDTR can be found in the Methods section
and SI. The measured in-plane thermal conductivity of 3C-SiC thin
films are lower than that of the bulk 3C-SiC crystal due to the size
effect. The measured in-plane \( \kappa \) values of 3C-SiC thin films at room
temperature are compared with that of other close-to-isotropic high
\( \kappa \) thin films such as AlN, diamond, and GaN (see Fig. 4b; strongly anisotropic materials graphite and h-BN have high in-plane \( \kappa \) values but
we do not include them here). The in-plane \( \kappa \) of 3C-SiC thin films show
record-high values, even higher than that of diamond thin films with
equivalent thicknesses. We attribute these high in-plane \( \kappa \) values to
the high-quality of the 3C-SiC thin films. These high in-plane \( \kappa \) values of 3C-
SiC thin films facilitate heat spreading of localized Joule-heating in
power electronics.

The cross-plane \( \kappa \) of the 3C-SiC thin films are measured by TDTR.
The dependence of cross-plane \( \kappa \) on film thickness and temperature are
shown in Fig. 4c, d. The measured cross-plane thermal conductivity
of 3C-SiC thin films are lower than that of the bulk 3C-SiC crystal due to
size effect. For the phonons in 3C-SiC with mean free paths longer than
the film thickness, the phonons scatter with the film boundaries which
cause reduction in the phonon mean free paths and corresponding
thermal conductivity. The cross-plane \( \kappa \) of 3C-SiC thin films are among
the highest values ever known, even higher than or comparable to that

(FWHM) of 158 arcsec. Both crystal quality and crystal purity affect
thermal conductivity. Both the high-purity and good crystal quality of
our 3C-SiC crystals result in the observed high \( \kappa \). The high \( \kappa \) in this work
validates the theory proposed in the literature that the abnormally low
\( \kappa \) observed in the literature is a consequence of the defective, poly-
crystalline quality of the 3C-SiC samples instead of the intrinsic prop-
erty of 3C-SiC.

To further prove that the B impurity reduces thermal conductivity
significantly as predicted by the theoretical paper, we grow an addi-
tional sample (3C-SiC film on Si substrate) which is intentionally doped
with B. The concentration of the intentional boron doping is \( 1 \times 10^{19} \) atoms cm\(^{-3} \) and the thickness of the 3C-SiC film is 1.87 \( \mu \)m. The mea-
sured thermal conductivity of this doped sample is 324 W m\(^{-1} \)K\(^{-1} \) which
is about 20% smaller than the un-doped 3C-SiC film with a similar
thickness (1.75 \( \mu \)m in the main text). This reduction in thermal con-
ductivity of 3C-SiC is consistent with the theoretical prediction in ref.
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}\text{nature communications}\mid (2022)13:7201
Fig. 3 | Temperature dependent $\kappa$ of bulk 3C-SiC crystals. a Comparison of the measured $\kappa$ in this work with previous measured $\kappa$ in the literature\textsuperscript{1,50,51}. The $\kappa$ value (red line) predicted by density functional theory (DFT) in this work is also included\textsuperscript{1,52}. The definition of error bars can be found in SI. b Comparison of temperature dependent $\kappa$ of 3C-SiC with c-axis $\kappa$ of bulk 6H-SiC, AlN, and GaN\textsuperscript{1,11,12}. The symbols are experimentally measured values while the lines are DFT-calculated values of perfect single crystals\textsuperscript{1,11}. We include both the cross-plane $\kappa$ and the in-plane $\kappa$ of 6H-SiC since its $\kappa$ is anisotropic.

Fig. 4 | High in-plane and cross-plane $\kappa$ of 3C-SiC thin films. a Beam-offset TDTR technique for in-plane $\kappa$ measurements. The out-of-phase TDTR signal on a 2.52-μm SiC on Si sample is shown as a function of beam offset distance. b In-plane $\kappa$ of 3C-SiC thin films. The $\kappa$ of 3C-SiC bulk crystal and the in-plane $\kappa$ of other close-to-isotropic high $\kappa$ thin films are also included for comparison\textsuperscript{32,53–59}. The definition of error bars can be found in SI. c Cross-plane $\kappa$ of 3C-SiC thin films. The $\kappa$ of 3C-SiC bulk crystal and cross-plane $\kappa$ of other high $\kappa$ thin films are also included for comparison\textsuperscript{20,23,27,40,53,48,59–61}. d Temperature dependent cross-plane $\kappa$ of a 1.75-μm-thick 3C-SiC thin film. The temperature dependent cross-plane $\kappa$ of AlN and GaN thin films are also included\textsuperscript{20,61}. 

Article https://doi.org/10.1038/s41467-022-34943-w Nature Communications | (2022) 13:7201 5
of diamond thin films with equivalent thicknesses. The cross-plane $\kappa$ of 1.75-µm-thick 3C-SiC reaches ~80% of the $\kappa$ of bulk 3C-SiC, up to twice as high as the $\kappa$ of bulk GaN. Even the 0.93-µm-thick 3C-SiC film has a cross-plane $\kappa$ close to that of bulk GaN. The different tendency of the thickness dependent thermal conductivity for different semiconductors are due to the different intrinsic phonon mean free path distributions in these semiconductors. The calculated phonon mean free path accumulated thermal conductivity of 3C-SiC scaled by the bulk thermal conductivity is compared with other semiconductors (see SI). It is notable that, since the epitaxial diamond thin films are polycrystalline, the grain boundaries and other structural imperfections also scatter phonons and affect the tendency of thermal conductivity as a function of film thickness. Figure 4d compares the temperature dependent cross-plane $\kappa$ of some wide-bandgap semiconductor thin films. In the measured temperature range, all the cross-plane $\kappa$ values of 3C-SiC are higher than that of AlN and GaN with even larger thicknesses. The high cross-plane $\kappa$, combined with the high in-plane $\kappa$, of these 3C-SiC thin films make them the best candidate for thermal management applications which use thin films.

The epitaxial growth of 3C-SiC not only produces high-quality thin films which have high in-plane and cross-plane $\kappa$ values, but also creates high-quality heterogeneous interfaces which are potentially thermally conductive. The cross-section TEM images of the epitaxial 3C-SiC-Si and 3C-SiC-AlN interfaces are shown in Fig. 5a, b to study the interfacial structure. Their TBC are measured by TDTR and compared with that of other semiconductor interfaces (Fig. 5c). All the interfaces are smooth interfaces with sub-nm roughness. Only the AlN-GaN interface is a bonded interface with a thin amorphous interfacial layer while all the other interfaces are fabricated by growing one semiconductor on top of the other well-polished semiconductor substrate. The measured 3C-SiC-Si TBC (~620 MW m$^{-2}$K$^{-1}$) is among the highest values for all interfaces making up of semiconductors, about ten times as high as that of the diamond-Si interfaces, about 2.5 times as high as that of epitaxial Si-Ge interfaces. It also approaches the maximum TBC of any interface involving Si, which is only limited by the rate that thermal energy in Si can impinge on the crystallographic plane. The measured 3C-SiC-AlN TBC is higher than the GaN-BAs TBC and 4H-SiC-GaN TBC. These high TBC values of 3C-SiC related interfaces facilitate heat dissipation of electronics and optoelectronics which use 3C-SiC, especially for the cases with an increasing number of interfaces as the minimization of devices.

In summary, this work reported an isotropic room-temperature high thermal conductivity exceeding 500 W m$^{-1}$K$^{-1}$ in high-purity wafer-scale free-standing 3C-SiC bulk crystals, which is ~50% higher than commercially available 6H-SiC and AlN. It is >50% higher than the previously measured $\kappa$ of 3C-SiC in the literature, and is the second highest among large crystals. We also studied the $\kappa$ of corresponding 3C-SiC thin films and found record-high in-plane and cross-plane $\kappa$ values. The measured higher $\kappa$ of 3C-SiC than that of the structurally more complex 6H-SiC validates that structural complexity and $\kappa$ are inversely related, resolving a long-standing puzzle about the perplexingly low $\kappa$ of 3C-SiC in the literature. Impurity concentrations measured by SIMS revealed the high-purity of our 3C-SiC crystals and the XRD measurements revealed the good crystal quality of our 3C-SiC crystals. Both contribute to the observed high $\kappa$. Furthermore, high TBC values were observed across epitaxial 3C-SiC-Si and 3C-SiC-AlN interfaces. The measured 3C-SiC-Si TBC is among the highest for semiconductor interfaces, about ten times as large as that of diamond-Si interfaces. The high $\kappa$ observed in 3C-SiC bulk crystals and thin films, combined with the high TBC of epitaxial 3C-SiC interfaces, suggest 3C-SiC an excellent candidate for applications of next-generation power electronics and optoelectronics. 3C-SiC has the best thermal (highest thermal conductivity) and electrical (highest channel mobility) properties among all SiC polytypes, and is a polyphtype which can be grown on Si which enables integration of 3C-SiC electronics with Si electronics with exceptionally high thermal boundary conductance.

**Methods**

**Samples**

The 3C-SiC samples in this work are acquired from Air Water Inc. and are available for purchase. The 3C-SiC crystals are grown on (111) Si substrates by low-temperature chemical vapor deposition (LT-CVD) in a customized CVD reactor at 1300 K. The orientation of the Si substrate and the growth temperature are important to grow high-quality crystals. Since both Si and 3C-SiC have the same rotational symmetry (120°) about the [111] axis, (111) 3C-SiC layers can be grown on (111) Si substrates with low density of stacking faults and double positioning boundary at relatively low crystal growth temperature (1300 K). The free-standing bulk 3C-SiC crystal is obtained by growing ~100-µm-thick 3C-SiC on Si substrates and then etching away the Si substrates by HNA (HF: HNO$_3$: H$_2$O). The stacking faults density observed on the growth face is about 1000 cm$^{-1}$ according to cross-sectional TEM study. The thermal conductivity of thermally thick 3C-SiC films grown on (100) Si purchased from MTI is only 90 W m$^{-1}$K$^{-1}$, which is significantly lower than that of our samples.

**Thermal characterizations**

The $\kappa$ and TBC are measured by time-domain thermoreflectance (TDTR). We coat ~90-nm-thick Al on the to-be-measured sample as TDTR transducer before TDTR measurements. TDTR is an ultra-fast laser based pump-probe technique which can measure thermal properties of both bulk and nanostructured materials. Modulated pump laser beam heats the sample surface periodically while a delayed probe laser beam detects the temperature variations of the sample surface via thermoreflectance. The signal picked up by a photodetector and a lock-in amplifier is fitted with an analytical heat
transfer solution of the sample structure to infer the unknown parameters (for example, \( \kappa \) of 3C-SiC and TBC of the metal transducer-SiC interface when measuring the 3C-SiC bulk crystals). We used 5× objective (spot size 10.7 \( \mu \)m) and 9.3 MHz when measuring the \( \kappa \) of the 3C-SiC bulk crystals and the cross-plane \( \kappa \) of 3C-SiC thin films. The growth face of the bulk 3C-SiC is polished and TDTR is performed on the growth face. When measuring the 3C-SiC thin films, the thicknesses of Al transducer and 3C-SiC thin films are measured by picosecond acoustic technique\(^{34} \). More details about the thickness measurements and used literature values of heat capacity can be found in SI. The in-plane \( \kappa \) of 3C-SiC thin films are measured by BO-TDTR with a modulation frequency of 1.9 MHz and an objective of 10×\(^{35} \). We also used the 5× objective to repeat the BO-TDTR measurements and obtained consistent results.

Raman spectroscopy

Raman measurements were performed on the 3C-SiC bulk crystal with a Horiba LabRAM confocal Raman spectroscopy imaging system. The used laser wavelength is 532 nm. The acquisition time is 600 s and the objective is 30×.

SIMS characterizations

The depth profiles of the O, N, and B atomic densities on the face close the Si substrate and the growth face were analyzed by secondary ion mass spectrometry (SIMS) (CAMECA: IMS-4f). An area of 150 \( \mu \)m \( \times \) 150 \( \mu \)m was sputtered with a beam of \( \mathrm{O}_2^+ \) beam accelerated at 8 keV to obtain the depth profile of the B atom density, an area of 220 \( \mu \)m \( \times \) 220 \( \mu \)m was sputtered with a beam of \( \mathrm{C}_6^+ \) beam accelerated at 14.5 keV to obtain the depth profiles of the O and N atomic densities.

STEM and SAED measurements

Scanning transmission electron microscopy (STEM) and selected area electron diffraction (SAED) (JEM-2200FS; JEOL) were used to analyze the crystal quality of the 3C-SiC crystals and the interfaces at an acceleration voltage of 200 kV. TEM samples were prepared by using a focused ion beam (FIB) system (Helios NanoLab 600i DualBeam; Thermo Fisher Scientific) by depositing a protective layer and milling using a 30 kV accelerating voltage, and final etching using a 2 kV accelerating voltage at room temperature.

XRD measurements

The crystal quality of the 3C-SiC crystals was characterized by the full width at half maximum on the X-ray rocking curve of the 3C-SiC (111) peak using an X-ray diffraction system (D8 Discover; Bruker). A Cu-Kα X-ray source accelerating at 40 kV with a current of 40 mA was applied to record the XRD patterns in the range of 17.2°–18.4° with a step of 0.015°. An incident slit with a width of 2 mm and a collimator with a diameter of 0.1 mm were used.

EBSD measurements

The crystal direction of the 3C-SiC crystals was analyzed by an Electron Backscatter diffraction (EBSD) system (FE-SEM JSM-6500F; JEOL) with a high-resolution scanning electron microscope (SEM) and a TSL orientation imaging microscopy (OIM) analyzer. The SEM was operated at 20 kV, and a scan area of 2.4 mm \( \times \) 0.8 mm was performed using a hexagonal grid with a step size of 2 \( \mu \)m. The EBSD measurements are done at Toray Research Center, Inc.

First-principle calculations

DFT simulations were performed by using the Vienna Ab initio simulation package (VASP) with the projector-augmented-wave method and the local density approximation (LDA) for exchange and correlation\(^{41} \). The plane-wave energy cutoff is selected as 500 eV. The primitive cell is relaxed with the energy convergence threshold of 10\(^{-6} \)eV/\( \text{Å}^2 \), force convergence threshold of 10\(^{-7} \)eV/\( \text{Å} \), and \( k \)-mesh of \( 15 \times 15 \times 15 \). The obtained lattice constant is 4.3306 Å. In the second-order and third-order force constants calculations, using Phonopy and ThirdOrder\(^{46,47} \), the supercell size is selected as \( 5 \times 5 \times 5 \) (250 atoms) with a \( 3 \times 3 \times 3 \) \( k \)-mesh and energy convergence threshold of 10\(^{-8} \)eV. The non-analytical correction that splits LO and TO phonons at \( \Gamma \) point is considered in the phonon dispersion calculations. Up to the 6th nearest neighbor of atoms are included in the third-order force constants extraction. The temperature-dependent thermal conductivity and phonon mean free path accumulated thermal conductivity are calculated by using ShengBTE using a 36 \( \times \) 36 \( \times \) 36 phonon \( q \)-mesh and a broadening factor of 0.1°. The calculation convergence regarding \( q \)-mesh and broadening factor is studied. Natural isotope-phonon scattering is included in the calculations.

Reporting summary

Further information on research design is available in the Nature Portfolio Reporting Summary linked to this article.

Data availability

The datasets generated during and/or analyzed during the current study are available from the corresponding authors upon reasonable request.

Code availability

The code used for calculations, simulations, and data analysis is available from the corresponding authors upon reasonable request.

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Acknowledgements
Z.C. and D.G.C. acknowledge the financial support from an endowed position created by the Grainger Engineering Breakthroughs Initiative. Z.C. and D.G.C. thank Guangxin Lyu for help of Raman measurements.
The fabrication of the TEM samples was performed at The Oarai Center and at the Laboratory of Alpha-Ray Emitters in IMR under the Inter-University Cooperative Research in IMR of Tohoku University (NO. 202112-IRKMA-0016). The observation of the TEM samples was supported by Kyoto University Nano Technology Hub in the “Nanotechnology Platform Project” sponsored by the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan. H.Z., J.T., and T.F. acknowledge the support from National Science Foundation (NSF) (award number: CBET 2212830). The computation used resources of the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231 using NERSC award BES-ERCAP0022132. The support and resources from the Center for High Performance Computing (CHPC) at the University of Utah and the Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS) of NSF are gratefully acknowledged. S.G. acknowledges the financial support from U.S. Office of Naval Research under a MURI program (Grant N00014-18-1-2429).

**Author contributions**
Z.C. initialized this project, developed the idea, and finished all the thermal measurements. Z.C. and J.L. coordinated the project. J.L. polished the bulk 3C-SiC samples and performed TEM studies. K.K., H.A., and H.U. grew the 3C-SiC samples and did XRD measurements. H.Z., J.T., and T.F. did the first principle calculations. Y.O. and Y.N. prepared the TEM FIB samples. Z.C. wrote the manuscript with inputs from all authors. J.L. assisted with manuscript preparation. S.G. and N.S. commented on the manuscript. D.G.C. provided overall guidance to the project and reviewed the manuscript.

**Competing interests**
K.K, H.A., and H.U. are employees of Air Water, Inc. which sells 3C-SiC related products. All the other authors declare no competing interest.

**Additional information**

**Supplementary information** The online version contains supplementary material available at https://doi.org/10.1038/s41467-022-34943-w.

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**Peer review information** Nature Communications thanks the anonymous reviewer(s) for their contribution to the peer review of this work. Peer reviewer reports are available.

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Supplementary Information

High Thermal Conductivity in Wafer-Scale Cubic Silicon Carbide Crystals

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Supplementary Note 1: EBSD measurements

The image quality (IQ) map and the crystal direction map are shown in Supplementary Fig. 1 (face close to Si substrate) and Supplementary Fig. 2 (growth face). The EBSD data in Supplementary Figs. 1 and 2 show that the 3C-SiC has single (111) crystal orientation over the entire scanned area (2.4 mm×0.8 mm) on both faces.

Supplementary Fig. 1. EBSD map of 3C-SiC from the face close to Si substrate. IQ map is the image quality map. The crystal direction map shows the spatial extent and amplitude of deviations of the orientations of the crystal (about 2 degree).
**Supplementary Fig. 2. EBSD map of 3C-SiC from the growth face.** IQ map is the image quality map. The crystal direction map shows the spatial extent and amplitude of deviations of the orientations of the crystal (about 2 degree).

**Supplementary Note 2: SIMS data**

The detailed second ion mass spectroscopy (SIMS) data is shown in Supplementary Fig. 3. The concentrations of O, N, and B are measured as a function of depth from the surface.
Supplementary Fig. 3. SIMS data of O, N, and B impurities. a data measured from the bottom side (close to the Si substrate). b data measured from the top side (growth side).

Supplementary Note 3: cross-plane $\kappa$ of 3C-SiC, 4H-SiC, and 6H-SiC

Supplementary Fig. 4 shows the comparison of the temperature dependent cross-plane $\kappa$ of 3C-SiC, 4H-SiC, and 6H-SiC bulk crystals. The thermal conductivity of 3C-SiC is higher than those of the 4H-SiC and 6H-SiC at all the reported temperatures.
Supplementary Fig. 4 Temperature dependent cross-plane κ of 3C-SiC, 4H-SiC, and 6H-SiC bulk crystals.

Supplementary Note 4: TDTR data fittings

The temperature dependent thermal conductivity and heat capacity of Si are from literature. The heat capacity data of 3C-SiC are the DFT-calculated values from Materials Project (DOI: 10.17188/1282015). Supplementary Fig. 5 shows the comparison of volumetric heat capacity of 3C-SiC, 4H-SiC, and 6H-SiC. The thicknesses of Al transducer and 3C-SiC films are determined by picosecond acoustic technique (see below for more details). The Al thermal conductivity is determined by measuring its electrical conductivity and applying Wiedemann-Franz law (170 W m⁻¹K⁻¹). The error bars of typical TDTR measurements are about ±10%.

Supplementary Fig. 5 Temperature dependent heat capacity of 3C-SiC, 4H-SiC, and 6H-SiC.
**Supplementary Note 5: Picosecond acoustic technique**

When the strain wave created by the pump laser reflects back from an interface, an echo shows up in the TDTR signal, as shown in Fig. S6. According to the delay time the strain wave travels in the film, we are able to measure the thickness of that film with known sound velocity. The sound velocity of 3C-SiC along [111] direction is 12.5 km/s. The sound velocity of Al is 6.4 km/s. The measured thicknesses of the 3C-SiC films are listed in Supplementary Fig. 6.

![Supplementary Fig. 6 Picosecond acoustic echoes of the 3C-SiC on Si samples with different 3C-SiC film thicknesses.](image)

**Supplementary Note 6: Beam offset TDTR**

The beam offset measurements were performed at a delay time of -50 ps with a 10× objective and a modulation frequency of 1.9 MHz. The measured full width at half maximum (FWHM) of the
out-of-phase TDTR signal as a function of beam offset distance in the beam offset experiments is fitted with the calculated FWHM values from analytical heat transport solution of the sample structure to obtain in-plane thermal conductivity of 3C-SiC films. Supplementary Fig. 7 shows an example of the data fitting process of a BO-TDTR measurement on the 2.52-μm-thick 3C-SiC thin films. The uncertainty of in-plane thermal conductivity due to the FWHM uncertainty is ±6 W m⁻¹K⁻¹, which is small compared to other errors in the experiment. The fitted in-plane thermal conductivity of the 3C-SiC film is 350±35 W m⁻¹K⁻¹. The sensitivity of the in-plane and cross-plane thermal conductivity of the 0.93-μm-thick 3C-SiC film is small so we report a ±20% error bar in this work.

Supplementary Fig. 7 Data fitting of BO-TDTR for the 2.52-μm-thick 3C-SiC thin films. The red circle is the fitted in-plane thermal conductivity with the measured FWHM. The measured full width at half maximum (FWHM) is from the out-of-phase TDTR signal as a function of beam offset distance in the beam offset experiments. The black line is the simulated values according to
the sample structure. The black dash lines are the uncertainties in the measurements of in-plane thermal conductivity as a result of the FWHM uncertainties (0.05 μm).

**Supplementary Note 7: TBC measurements**

TDTR is performed on the 1.75 μm and 0.93 μm 3C-SiC on Si samples to measure the 3C-SiC-Si TBC. The data fittings of the TDTR ratio and fitted results are shown in Supplementary Fig. 8. Consistent 3C-SiC-Si TBC values are obtained in both measurements (~620 MW m⁻²K⁻¹). Similar measurements are also performed on the 2.52 μm 3C-SiC on Si sample but it is insensitive to the 3C-SiC-Si TBC because of the large thickness.

![Supplementary Fig. 8 TDTR ratio fitting of the measurements.](image)

**Supplementary Fig. 8 TDTR ratio fitting of the measurements.** a 1.75 μm 3C-SiC on Si sample with 5x and 9.3 MHz. b 0.93 μm 3C-SiC on Si sample with 5x and 9.3 MHz. The circles are experimental data while the red lines are the fitting curves. The fitted results are also included.
To further check the fitted data in the Supplementary Fig. 8, we force the 3C-SiC-Si TBC as a certain value close to 620 MW m$^{-2}$K$^{-1}$ and refit the $\kappa$ of the 3C-SiC thin films. The relation between the 3C-SiC-Si TBC and the $\kappa$ of the 3C-SiC thin films are shown in Supplementary Fig. 9. The empty circles are the first set of measurements while the filled circles are repeating data collected on different spots on corresponding samples. Due to size effect, thicker film has higher thermal conductivity. Here, 2.52-μm-thick 3C-SiC film should have higher $\kappa$ than that of the 1.75-μm-thick 3C-SiC film. According to Supplementary Fig. 9, the 3C-SiC-Si TBC needs to be higher than 500 MW m$^{-2}$K$^{-1}$. The measured 3C-SiC-Si TBC (620 MW m$^{-2}$K$^{-1}$) agrees with the measurements on these three samples. Thus, the best-fit value of the 3C-SiC-Si TBC is 620 MW m$^{-2}$K$^{-1}$ with a lower limit of 500 MW m$^{-2}$K$^{-1}$.

Supplementary Fig. 9. Refitting TDTR data of the three 3C-SiC on Si samples. The $\kappa$ of the 3C-SiC thin films are fitted by forcing the 3C-SiC-Si TBC as a certain value. There are two sets of data points which are measured on different spots on the corresponding samples.
Supplementary Note 8: XRD FWHM

Supplementary Fig. 10 shows the full width at half maximum (FWHM) of SiC (111) peak in the rocking curve of X-ray diffraction on the 3C-SiC thin films as a function of film thickness grown on Si substrates. The data of NovaSiC and Matsunami are from literature. The lower values of FWHM of our samples than literature values show the improved quality of 3C-SiC crystals. As the films grow thicker, the FWHM values decrease. The 3C-SiC near the 3C-SiC-Si interfaces have relatively low crystal quality while the quality improves as the films grow thicker.

Supplementary Fig. 10 The full width at half maximum of SiC (111) peak in the rocking curve of X-ray diffraction on the 3C-SiC thin films as a function of film thickness grown on Si substrates. Air water is our sample source in this work. The data of NovaSiC and Matsunami are from literature.
Supplementary Note 9: 3C-SiC-AlN interfaces

To measure the TBC of 3C-SiC-AlN interfaces, the sample was fabricated as shown in Supplementary Fig. 11. A layer of 1 μm 3C-SiC is grown on a Si substrate before epitaxial growth of AlN and GaN layers. Then the GaN is bonded to a Si template before etching away the Si substrate. After polishing the exposed 3C-SiC surface, a layer of Al is coated as TDTR transducer. The thickness of 3C-SiC layer is 887 nm and the AlN layer is 2530 nm. In TDTR measurements, only the Al layer, 3C-SiC layer, and the AlN layer are considered in the data fitting since AlN is thermally thick with a modulation frequency of 9.3 MHz. The thermal conductivity of AlN layer used 200 W m⁻¹ K⁻¹ in the data fitting by referring to literature values of epitaxial AlN films.⁸⁹ The reported TBC value in the main text is the best-fit value.

Supplementary Fig. 11. Sample fabrication for TBC measurements of 3C-SiC-AlN interfaces.

The STEM study of the 3C-SiC-AlN interfaces are shown in Supplementary Fig. 12. The FFT data of AlN is shown in Supplementary Fig. 12a while the orientations and lattice constants of both AlN and 3C-SiC are shown in Supplementary Fig. 12b.
Supplementary Fig. 12 STEM study of the 3C-SiC-AlN interfaces. a Fast Fourier transform (FFT) of the STEM image of the AlN. b Orientations and lattice constants of AlN and 3C-SiC.

Supplementary Note 10: First principle calculations

Supplementary Fig. 13. First principle calculated thermal conductivity of perfect single crystal 3C-SiC.
Supplementary Fig. 14. Calculated phonon properties of perfect 3C-SiC single crystal. a Phonon dispersion relation of perfect 3C-SiC single crystal. b Accumulated thermal conductivity of perfect 3C-SiC single crystal at 300, 400, and 500 K. It shows the contributions of phonons with different mean free paths to the total thermal conductivity.
Supplementary Fig. 15. The accumulated thermal conductivity of 3C-SiC, AlN, GaN, and diamond scaled by their bulk thermal conductivity at room temperature.

Supplementary Note 11: Laser information

The Raman measurements and TDTR measurements use lasers. The laser information of the Raman system can be found in the product manual (Horiba LabRAM). The TDTR laser is a Spectra-Physics pulsed Ti-sapphire Tsunami laser. Detailed information can be found in the product manual.
Supplementary Table 1. The list of thermal conductivity of nanocrystalline diamond thin films and the corresponding references.

| Thickness [μm] | $k_{\text{in-plane}}$ [W m⁻¹ K⁻¹] | $k_{\text{out}}$ [W m⁻¹ K⁻¹] | References |
|---------------|-------------------------------|-------------------------------|------------|
| 1.06          | 117                           |                               | 10         |
| 3.02          | 157                           |                               | 10         |
| 1.1           | 95                            | 175                           | 11         |
| 1             | 103                           |                               | 12         |
| 0.47          | 40                            |                               | 13         |
| 0.475         | 90                            |                               | 13         |
| 0.68          | 65                            |                               | 13         |
| 1             | 75                            |                               | 13         |
| 1             | 85                            |                               | 13         |
| 1             | 130                           |                               | 13         |
| 0.98          | 145                           |                               | 13         |
| 1.5           | 190                           |                               | 13         |
| 0.5           | 52                            |                               | 14         |
| 1             | 77                            | 210                           | 14         |
| 5.6           | 130                           | 710                           | 14         |
| 2             |                               | 280                           | 15         |
| 2             |                               | 310                           | 15         |
| 2             |                               | 360                           | 15         |
| 5             |                               | 703                           | 16         |
| 1             | 93                            | 180                           | 17         |
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