Solving the puzzle: Cubic silicon carbide wafer demonstrates high thermal conductivity, second only to diamond

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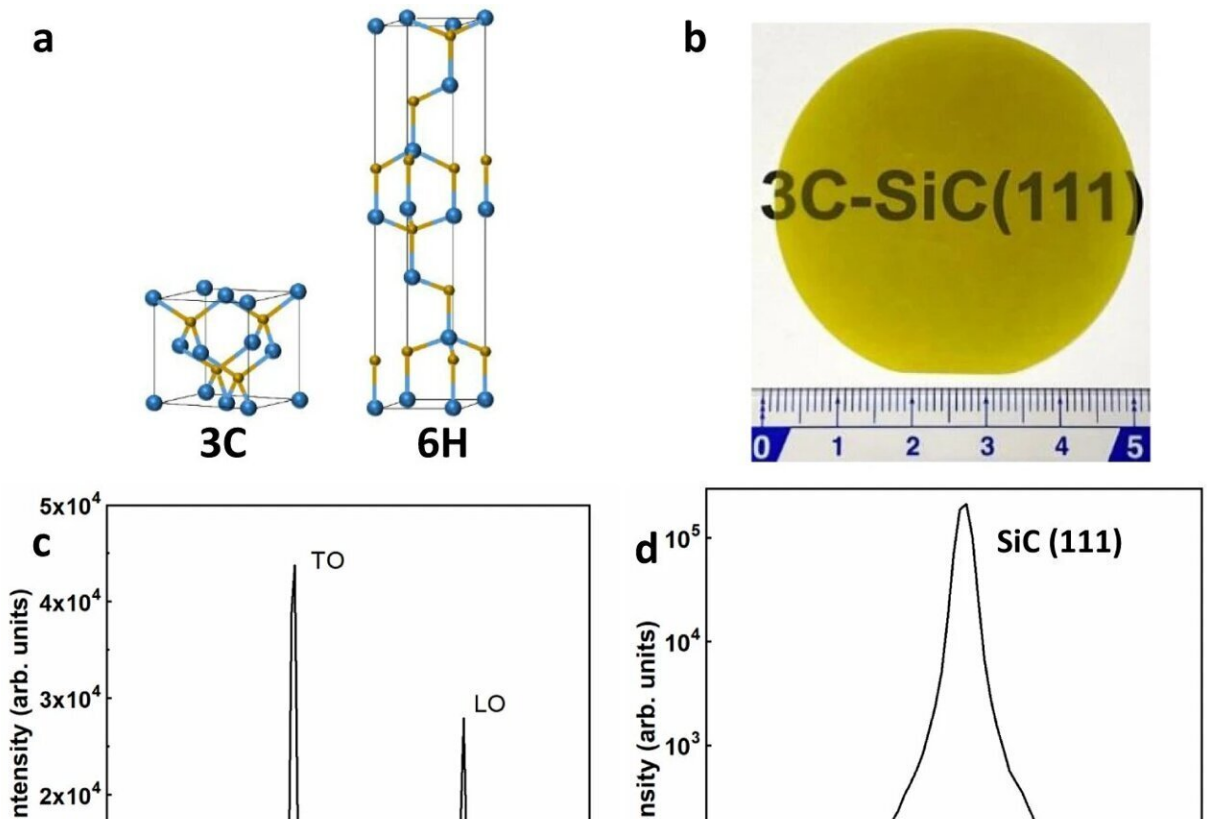

Structure of wafer-scale free-standing 3C-SiC bulk crystals. a Atomic structures of 3C-SiC and 6H-SiC. b Picture of a 3C-SiC 2-inch wafer. The unit of the ruler is cm. c Raman spectrum of 3C-SiC crystal. d X-ray diffraction (XRD) of 3C-SiC. e High-resolution STEM image of 3C-SiC taken along the [110] zone axis. The inset: Fast Fourier transform (FFT) of the STEM image. f Selected area electron diffraction pattern of 3C-SiC taken in the [110] zone axis. Credit:

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A team of University of Illinois Urbana-Champaign Material Science and Engineering researchers have solved a long-standing puzzle about lower measured thermal conductivity values of cubic silicon carbide (3C-SiC) bulk crystals in the literature than the structurally more complex hexagonal phase SiC polytype (6H-SiC). The new measured thermal conductivity of bulk 3C-SiC has the second highest thermal conductivity among inch-scale large crystals, second only to diamond.

Professor David Cahill (Grainger Distinguished Chair in Engineering and co-director of the IBM-Illinois Discovery Accelerator Institute) and Dr. Zhe Cheng (Postdoc) report an isotropic high thermal conductivity of 3C-SiC crystals that exceeds 500 W $m^{-1}K^{-1}$. The team collaborated with Air Water, Inc, based in Japan, to grow high-quality crystals, with the thermal conductivity measurements performed at UIUC in the MRL Laser and Spectroscopy suite. Their results were recently published in *Nature Communications.*

Silicon carbide (SiC) is a wide bandgap semiconductor used commonly in electronic applications and has various crystalline forms (polytypes). In power electronics, a significant challenge is thermal management of high localized heat flux that can lead to overheating of devices and the degradation of device performance and reliability in the long-term. Materials with high thermal conductivity (κ) are critical in thermal management design.

Hexagonal phase SiC polytypes (6H and 4H) are the most widely used and extensively studied, whereas the cubic phase SiC polytype (3C) is less understood, despite it having the potential to have the best electronic properties and higher κ. Cahill and Zhe explain that there has been a long-standing puzzle about the measured thermal conductivity of 3C-SiC in the literature: 3C-SiC is lower than that of the structurally more complex 6H-SiC phase and measures lower than the theoretically predicted κ value.

This is a contradiction of predicted theory that structural complexity and thermal conductivity are inversely related (as structural complexity goes up, thermal conductivity should go down).

Zhe says that 3C-SiC is "not a new material, but the issue researchers have had before is poor crystal quality and purity, causing them to measure lower thermal conductivity than other phases of silicon carbide." Boron impurities contained in the 3C-SiC crystals cause exceptionally strong resonant phonon scattering, which significantly lowers its thermal conductivity.

Wafer-scale 3C-SiC bulk crystals produced by Air Water Inc. were grown by low-temperature chemical vapor deposition and had high crystal quality and purity. The team observed high thermal conductivity from the high purity and high crystal quality 3C-SiC crystals.

Zhe says that "the measured thermal conductivity of 3C-SiC bulk crystals in this work is ~50% higher than the structurally more complex 6H-SiC, consistent with predictions that structural complexity and thermal conductivity are inversely related. Moreover, the 3C-SiC thin films grown on Si substrates have record-high in-plane and cross-plane thermal conductivities, even higher than that of diamond thin films with equivalent thicknesses."

The high thermal conductivity measured in this work ranks 3C-SiC second to single crystal diamond among inch-scale crystals, which has the highest κ among all natural materials. However, for thermal management materials, diamond is limited by its high cost, small wafer size, and difficulty in integration with other semiconductors.

3C-SiC is cheaper than diamond, can easily be integrated with other materials, and can be grown to large wafer sizes, making it a suitable thermal management material or an excellent electronic material with a high thermal conductivity for scalable manufacturing.

Cahill says, "The unique combination of thermal, electrical, and structural properties of 3C-SiC can revolutionize the next generation of electronics by using it as active components (electronic materials) or thermal management materials," since 3C-SiC has the highest thermal conductivity among all SiC polytypes and helps facilitate device cooling and reduce power consumption.

The high thermal conductivity of 3C-SiC has potential to impact applications such as power electronics, radio-frequency electronics, and optoelectronics.

More information: Zhe Cheng et al, High thermal conductivity in wafer-scale cubic silicon carbide crystals, *Nature Communications* (2022). DOI: 10.1038/s41467-022-34943-w

Provided by University of Illinois Grainger College of Engineering

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