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θ -TaN: Redefining the thermal conductivity limit of metallic materials

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The relentless drive towards smaller, faster, and more powerful electronics has made thermal management a critical bottleneck for performance and reliability. For over a century, the thermal conductivity (κ) of metallic materials has long been considered to have an inherent upper limit for thermal conductivity, plateauing $\sim 400 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$. This ceiling is rooted in fundamental physics: in typical metals, heat is primarily carried by electrons, and their transport is severely hampered by strong electron–phonon coupling and inherent lattice anharmonicity^[1]. These intrinsic scattering mechanisms have historically confined the thermal performance of metals. This limit has posed a critical bottleneck for advanced electronics, where escalating power densities (projected to reach $1 \text{ MW}/\text{cm}^2$ by 2030) demand more efficient heat dissipation^[2].

However, a groundbreaking study published in *Science* (*Science* (2026), doi:10.1126/science.aeb1142)^[3] by Li *et al.* shatters this barrier through the experimental realization of single-crystalline θ -phase tantalum nitride (θ -TaN), a metastable transition metal nitride with a room-temperature thermal conductivity of $\sim 1100 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$, nearly three times that of copper. This work not only validates decades of theoretical predictions^[4–6] but also introduces a new class of high-thermal-conductivity metals, opening transformative opportunities for thermal management in electronics, aerospace, and energy systems.

For decades, the quest for ultrahigh thermal conductivity has been focused on semiconductors and insulators like diamond, cubic boron nitride, and more recently, boron arsenide (BAs)^[7, 8]. These materials exploit high sound velocities, strong covalent bonding, and low atomic mass to achieve phonon-dominated heat transport exceeding $1000 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$. Metals, in contrast, were seemingly boxed in by their very nature. Their excellent electrical conductivity comes at the cost of strong interactions between the charge-carrying electrons and the lattice vibrations (phonons). This electron–phonon coupling acts as a dominant scattering mechanism, curtailing the mean free paths of both carriers and capping the total κ ^[1]. The recent success of BAs, with its κ rivaling diamond, demonstrated that breaking conventional guide-

lines (like low average atomic mass) was possible through unique phonon band structure engineering, specifically, a large acoustic-optical phonon gap and bunching of acoustic branches to suppress phonon–phonon scattering^[7, 8]. This raised a tantalizing question: could similar principles be applied to a metallic system, effectively decoupling electron and phonon transport to achieve unprecedented κ ?

Theoretical work, notably the 2021 prediction by Kundu *et al.*, suggested that θ -TaN might be the answer^[4]. The key to θ -TaN's exceptional performance lies in its hexagonal crystal structure (space group $P6m2$) (Fig.1(a)), where tantalum and nitrogen form rigid, interpenetrating covalent networks. This metastable phase was calculated to possess a rare combination of properties: a large acoustic-optical gap, significant acoustic phonon bunching, exceptionally weak electron–phonon coupling due to its specific electronic structure, and minimal isotope scattering thanks to the near-monoisotopic nature of tantalum (^{181}Ta , 99.988%). Together, these features were predicted to grant θ -TaN a phonon-dominated thermal conductivity approaching $1000 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$. The challenge, however, lay in the synthesis. The θ phase is metastable and competes with several other TaN polymorphs. Previous attempts often yielded polycrystalline, defective samples where grain boundaries and impurities masked the intrinsic properties, resulting in measured κ values far below predictions^[9].

The breakthrough by Li *et al.* was their innovative synthesis strategy^[3]. They employed a flux-assisted metathesis reaction using sodium, which acted as both a reducing agent and a flux to facilitate the nitridation of tantalum oxides in a nitrogen-rich environment. This method circumvented the extreme high-pressure, high-temperature routes and yielded high-quality, faceted single crystals ranging from 10 to $100 \mu\text{m}$ in size. The authors synthesized high-quality single crystals using a flux-assisted metathesis reaction, overcoming the challenges of conventional high-pressure routes to minimize defects, grain boundaries, and mixed phases, all of which degrade transport properties^[9]. Structural validation via Raman spectroscopy (Fig.1(b)), single-crystal X-ray diffraction (Fig.1(c)), and high-resolution transmission electron microscopy confirms the material's phase purity, long-range order and uniform atomic distribution of Ta and N, laying the foundation for its intrinsic thermal behavior.

With high-quality crystals in hand, the team employed the time-domain thermoreflectance technique to measure thermal conductivity^[3]. The results were striking: a room-tempera-

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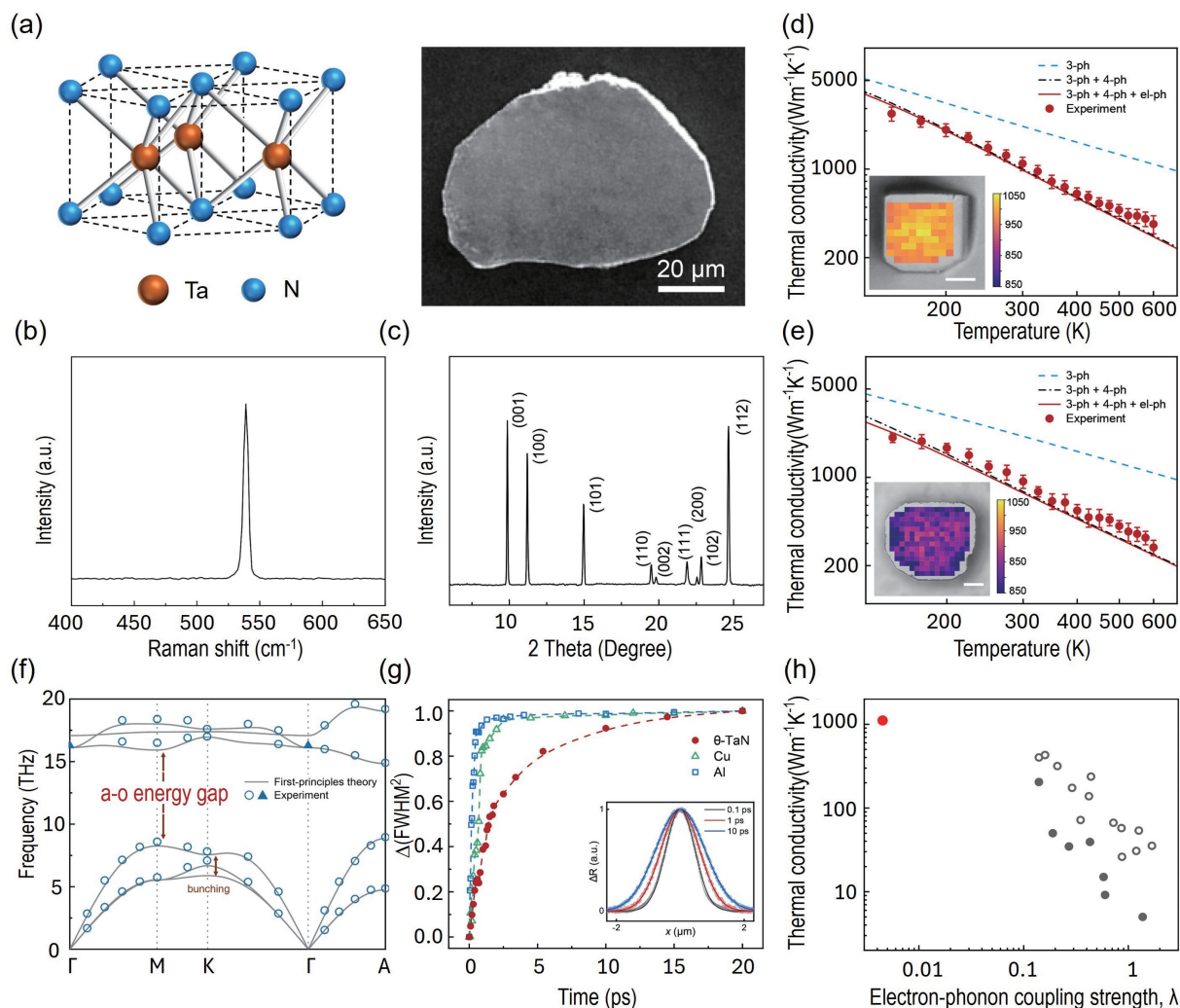


Fig. 1. (Color online) Schematic of θ -Ta N 's structure and thermal transport mechanisms. (a) Hexagonal crystal structure of θ -Ta N and scanning electron microscope image of a θ -Ta N crystal. (b) Raman spectroscopy of θ -Ta N . (c) Single X-ray diffraction spectrum. Measured thermal conductivity of θ -Ta N (red dots) along the (d) a -axis and (e) c -axis in comparison to first-principles calculations. Insets indicate the spatial mapping of thermal conductivity across the θ -Ta N crystals. (f) Phonon band structure measured via IXS (circles) and first-principles calculations (solid lines). (g) Time-dependent electron relaxation profiles measured for θ -Ta N (red, circles), Cu (green, triangle), and Al (blue, square). (h) Thermal conductivity versus electron-phonon coupling strength (λ) of θ -Ta N and conventional metals, highlighting its exceptionally weak electron-phonon coupling^[3].

ture κ of $1105 \pm 134 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ along the a -axis (Fig. 1(d)) and $928 \pm 111 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ along the c -axis (Fig. 1(e)). Spatially resolved mapping showed uniform values across the crystals, confirming the intrinsic nature of this ultrahigh conductivity. Crucially, the temperature dependence of κ exhibited a marked decrease with increasing temperature, a signature of phonon-dominated heat transport. This is distinct from the weak temperature dependence typical of electron-dominated metals like copper. Despite θ -Ta N 's metallic electrical conductivity ($\sim 1.5 \times 10^6 \text{ S}\cdot\text{m}^{-1}$), the Wiedemann-Franz law estimate confirmed that the electronic contribution to κ was minor, underscoring the primacy of phonons.

To unravel the microscopic origins, Li *et al.* turned to unravel this phenomenon using synchrotron-based inelastic X-ray scattering to map the phonon band structure of θ -Ta N (Fig. 1(f)). Two critical features emerge: a large acoustic-optical phonon gap ($\sim 8 \text{ THz}$) that suppresses scattering between acoustic (heat-carrying) and optical modes, and acoustic phonon bunching, where transverse and longitudinal acoustic branches remain tightly clustered in energy. The gap

severely restricts scattering events between heat-carrying acoustic phonons and optical phonons, while the bunching narrows the phase space for scattering among acoustic phonons themselves. First-principles calculations of scattering rates decomposed the contributions, showing that three-phonon processes, though dominant, are significantly suppressed in the crucial mid-to-high frequency acoustic range (6–8 THz) due to these phonon band structure features. This suppression amplifies the relative role of higher-order four-phonon scattering. Isotope scattering was negligible, as expected from Ta's isotopic purity. The combination of these effects extends phonon lifetimes.

Complementary ultrafast optical spectroscopy confirms exceptionally weak electron-phonon coupling in θ -Ta N ($\lambda \approx 0.0045$ at 300 K) (Fig. 1(g)), far lower than in typical metals (Fig. 1(h))^[10–12]. Hot electron relaxation measurements reveal a prolonged relaxation time of $\sim 15 \text{ ps}$, an order of magnitude longer than copper or aluminum, providing direct experimental evidence of minimal electron-phonon scattering. First-principles calculations further validate these findings,

showing that electron–acoustic phonon coupling is negligible near the Fermi level, while the large phonon gap restricts indirect energy transfer via optical phonons. This weakness is attributed to θ -TaN's specific electronic structure arising from direct d – d bonding between Ta atoms, resulting in a semimetallic character with a low electronic density of states at the Fermi level^[4]. The result is a material that retains metallic electrical conductivity while leveraging phonon transport to achieve ultrahigh thermal conductivity.

The discovery of θ -TaN redefines the design principles for high-thermal-conductivity materials. It demonstrates that the thermal conductivity of metals is not fundamentally limited to $\sim 400 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$. By strategically designing materials with specific phononic band structures (large gaps, bunching), weak electron–phonon coupling, and low isotopic disorder, it is possible to unlock phonon-dominated heat transport in metallic systems. θ -TaN, combines metallic behavior with phonon-dominated heat transport, making it uniquely suited for applications requiring both electrical connectivity and efficient cooling, such as AI accelerators, power semiconductors, and aerospace components. Additionally, its synthesis via a scalable flux-assisted method raises the prospect of industrial adoption, avoiding extreme pressure and temperature conditions.

Li *et al.*'s work^[3] opens new avenues for materials research. The success of θ -TaN suggests that metastable transition metal nitrides and carbides may harbor similar properties, as theoretical predictions have indicated for tungsten carbide and other compounds^[11]. Future efforts could focus on optimizing synthesis to scale up crystal size, exploring alloying to tune thermal and electrical properties, and integrating θ -TaN into device architectures to demonstrate real-world performance.

Moreover, the study highlights the power of combining advanced characterization techniques, such as IXS, ultrafast spectroscopy and high-resolution microscopy, with first-principles calculations to unravel complex transport phenomena. It provides a validated blueprint for discovering new high- k materials, particularly in the underexplored landscape of metallic and semimetallic compounds. This multimodal approach could accelerate the discovery of other materials that break conventional limits, addressing pressing needs in thermal management, thermoelectrics, and energy conversion.

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