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Large phonon-drag thermopower polarity reversal in Ba-doped KTaO₃

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This study reports the observation of phonon-drag thermopower polarity reversal in Ba-doped KTaO₃ thin films, mediated by electron-phonon Umklapp scattering. Epitaxial films with distinct carrier concentrations ($3.3 \times 10^{18} \text{ cm}^{-3}$, $4.9 \times 10^{19} \text{ cm}^{-3}$, and $3.7 \times 10^{20} \text{ cm}^{-3}$) were grown via molecular-beam epitaxy. In the heavily doped sample, where the Fermi surface spans 80% of the Brillouin zone in some directions, the Umklapp condition is satisfied, reversing electron momentum. This manifests as a sign-reversal in the thermopower around 80 K upon cooling despite the sample having only n-type carriers. On the other hand, the lightly doped samples (3.3×10^{18} and $4.9 \times 10^{19} \text{ cm}^{-3}$) exhibit only a negative thermopower down to 2 K. These results advance the understanding of Umklapp electron-phonon-drag in oxides and highlight KTaO₃'s potential for engineering unconventional thermoelectric materials.

The quest for materials with high thermoelectric efficiency at low temperature has recently resulted in thermoelectric figures of merit exceeding 2.5¹. Achieving high thermoelectric performance requires enhancement of the Seebeck coefficient, which can be accomplished through various mechanisms, including the use of 1-dimensional features¹, but also phonon-drag^{2–7}. Phonon-drag is an electronic transport phenomenon in which the electron population in a crystal interacts with its phonon population in a manner intense enough that both populations are brought outside thermodynamic equilibrium. This results in a strong enhancement of the Seebeck coefficient over its value in the diffusion regime, where both populations remain in equilibrium. For this to happen, the electron-phonon interactions must be stronger (i.e., have a shorter relaxation time) than the ubiquitous phonon-phonon interactions. Phonon-drag typically results in a boost in thermopower that has a non-monotonic temperature dependence. At temperatures below a maximum that is roughly at the Debye temperature divided by 5, it increases with the increase in phonon population upon warming. At temperatures above that maximum, it decreases as phonon-phonon Umklapp scattering becomes dominant over phonon-electron interactions. In almost all metallic crystals in which conduction is dominated by charge carriers of a single polarity (thus excluding semimetals), the phonon-drag thermopower has the same sign as the diffusion thermopower. The latter is also directly related to the polarity of the charge carrier in most single-polarity metallic solids (except Cu, Ag, Au, and Li, metals in

which the Fermi surface is topologically not simply-connected, which gives a positive diffusion thermopower even though the conduction is via electrons)⁸, i.e., electrons give a negative diffusion thermopower and holes a positive one. There is only one known case where the phonon-drag thermopower and the diffusion thermopower have opposite signs: Rb⁹. In this work, we report a change in polarity between the diffusion and phonon-drag thermopowers of heavily doped KTaO₃ (KTO) films.

The observed change in polarity is attributed to electron-phonon Umklapp scattering. Conventionally, Umklapp (U) scattering is known to play an important role in 3-phonon interaction processes, where it then strongly affects the lattice thermal conductivity. What is much less appreciated is that it also exists for electron-phonon interactions, a fact that is belied by the results presented here. In Normal (N) electron-phonon scattering processes, the change in the electron momentum is equal to that gained by the phonon. When the wave vectors of the interacting electron (**k**) and phonon (**q**) are small, the **k**-vector of the scattered electron (**k'**) is given by:

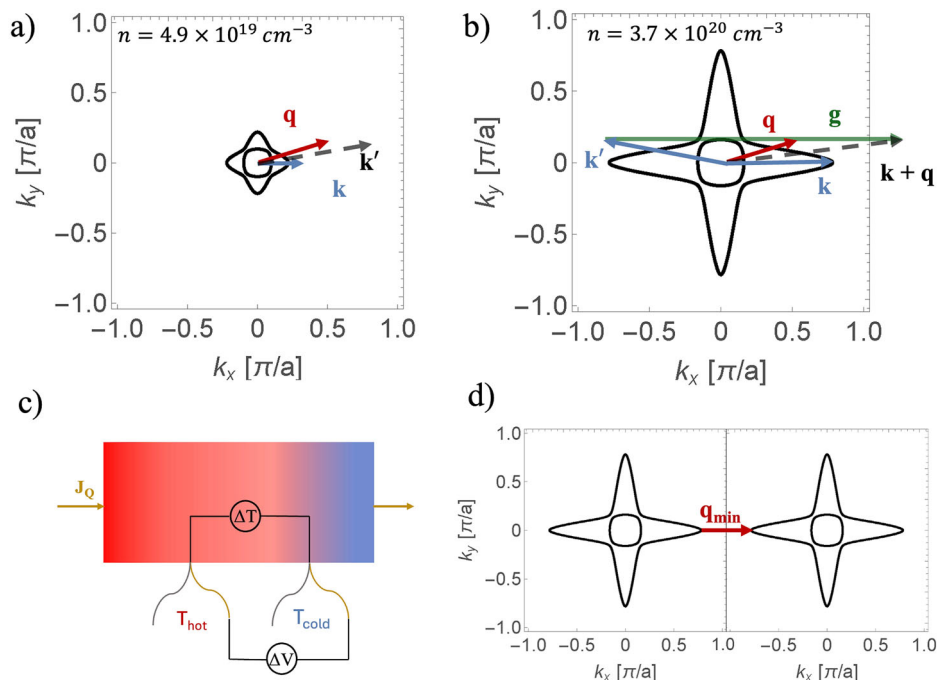
$$\mathbf{k}' = \mathbf{k} + \mathbf{q} \quad (1)$$

and **k'** still falls in the same Brillouin zone (BZ), and its sign is the same as that of **k** (Fig. 1a). U-scattering arises when **k** is large enough so that **k** + **q** falls in the next BZ, which happens when $|\mathbf{k} + \mathbf{q}| > |\mathbf{g}|/2$, where **g** is the

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Fig. 1 | The Seebeck effect was measured on KTaO₃ thin films with various carrier concentrations to determine how the size of the Fermi surface occupying the Brillouin zone affects the phonon-electron interactions and scattering events.

a Normal and **b** Umklapp conditions for electron-phonon scattering. Calculated 2D cuts in the (k_x, k_y) plane of the 3D Fermi surfaces for electron-doped KTaO₃ with carrier concentrations, $4.9 \times 10^{19} \text{ cm}^{-3}$ in **(a)** and $3.7 \times 10^{20} \text{ cm}^{-3}$ in **(b)**. A “thermal phonon” of energy $k_B T$ and momentum $\mathbf{q}$ interacting with an electron on the Fermi surface of momentum $\mathbf{k}$ does not fulfill the condition for Umklapp scattering in **(a)** but does in **(b)**. The resulting electron momentum $\mathbf{k}'$ moves in the same direction as $\mathbf{k}$ in **(a)** but in the opposite direction in **(b)**, where it gives a phonon-drag Seebeck coefficient of polarity opposite to that of the charge carrier. **c** A schematic of the sample mount and the direction of the applied temperature gradient. The minimum phonon momentum that satisfies the condition for U-phonon-drag is $\mathbf{q}_{\min}$ shown in **(d)**.



reciprocal lattice vector. Now:

$$\mathbf{k}' = \mathbf{k} + \mathbf{q} - \mathbf{g} \quad (2)$$

where $\mathbf{k}'$ undergoes a Bragg reflection, leading to a large change of momentum characterized by the vector $\mathbf{g}$ (Fig. 1b). In the diffusive regime, both N and U electron-phonon scattering processes are resistive, and differentiating between them is not critical to either resistivity or thermopower. In the case of U-phonon-drag processes, the resulting electron ($\mathbf{k}'$) will have a momentum opposite to both electrons and phonons due to the Bragg reflection. This manifests itself by generating a Seebeck coefficient of polarity opposite to that of the charge carrier.

While this mechanism was speculated to be true in Rb¹⁰, which has a constant electron density, the present paper offers a more convincing argument, since the doping level of the KTaO₃ films can be changed, allowing for a change in $\mathbf{k}$. In this work, we present three different Ba-doped KTaO₃ thin films with different carrier concentrations, $3.3 \times 10^{18} \text{ cm}^{-3}$, $4.9 \times 10^{19} \text{ cm}^{-3}$ and $3.7 \times 10^{20} \text{ cm}^{-3}$ with thicknesses of 100 nm, 70 nm and 100 nm, respectively.

There is no change in sign between diffusion and phonon-drag thermopower in lightly doped KTO, where the Fermi surface (Fig. 1a) is small and $|\mathbf{k} + \mathbf{q}| < |\mathbf{g}|/2$. In contrast, there is one in the heavily doped material, where the condition $|\mathbf{k} + \mathbf{q}| > |\mathbf{g}|/2$ is met (Fig. 1b).

For completeness, we mention the case of PdCoO₂, where a positive diffusion thermopower is accompanied by a negative phonon-drag thermopower¹¹. Nevertheless, that highly anisotropic material deviates strongly from a simple metal, and the in-plane thermopower is positive while the out-of-plane one is negative¹², making it a goniopolar material¹³.

KTaO₃ is an incipient ferroelectric that retains a cubic structure ($m\bar{3}m$) down to low temperatures^{14,15}. Stoichiometric KTaO₃ is an insulator with a bandgap of $\sim 3.6 \text{ eV}$, separating oxygen 2p-derived valence band from tantalum 5d-derived conduction band¹⁶. Due to strong spin-orbit coupling, the six-fold degeneracy of the conduction band's t_{2g} states at the zone center is lifted, resulting in a splitting into total angular momentum states $J = 3/2$ and $J = 1/2$ ¹⁷. In doped KTaO₃, itinerant electrons occupy the lower-energy $J = 3/2$ states, which split into two doubly degenerate bands at finite momentum (depicted as inner and outer bands in Fig. 1).

KTaO₃ hosts a wide variety of exotic emergent phenomena and properties, including an anisotropic superconducting state that is remarkably resilient to applied magnetic fields^{18–20}, non-trivial quantum geometrical effects^{21–24}, and efficient spin-to-charge interconversion^{25,26}. These properties are typically probed using magneto-electric experiments. The thermoelectric transport behavior of electron-doped KTaO₃ has been explored in bulk materials but not in thin films²⁷.

Results and discussion

Material characterization

The results for the X-Ray Diffraction (XRD) measurements are shown in Fig. 2a. Also shown are the characterization of the samples by Hall measurements (Fig. 2b, c). In particular, the samples grown on the KTaO₃ (100) substrate had carrier concentrations (n) of $3.7 \times 10^{20} \text{ cm}^{-3}$ and $3.3 \times 10^{18} \text{ cm}^{-3}$ and carrier mobility of $5.18 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ and $6.68 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, while the one grown on TbScO₃ (110)_o had a carrier concentration of $\sim 4.9 \times 10^{19} \text{ cm}^{-3}$ and carrier mobility of $14.71 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at 100 K.

Thermoelectric transport

The Seebeck effect is shown in Fig. 3a for the three samples. The diffusion thermopower, measured at $T > 100 \text{ K}$, is negative for all the samples, with an absolute value that is nearly linear in T , as expected for an n -type degenerately-doped semiconductor. The non-monotonic temperature-dependence points to the existence of phonon-drag below 100 K for the sample grown on KTaO₃ with carrier concentration of $3.7 \times 10^{20} \text{ cm}^{-3}$ and below 20 K for the one grown on TbScO₃ (110)_o with carrier concentration of $4.9 \times 10^{19} \text{ cm}^{-3}$. Unexpectedly, the data for the sample on KTaO₃ displays a positive thermopower below $\sim 80 \text{ K}$ even though there are no holes present in the system. As explained in the introduction, this peculiar observation points to the addition of unexpected scattering events that reverse the momentum direction of the electrons.

The presence of electron-phonon U-phonon-drag depends on a few factors: size of the Fermi surface, the mode-and-energy dependent phonon density, and the defects in the system. For phonon-drag to occur, the scattering between phonons and electrons of the system needs to be more intense than all other phonon scattering mechanisms, particularly phonon-defect and phonon-phonon scattering. The latter condition implies that phonon-drag occurs at lower temperatures, typically one-fifth of the Debye

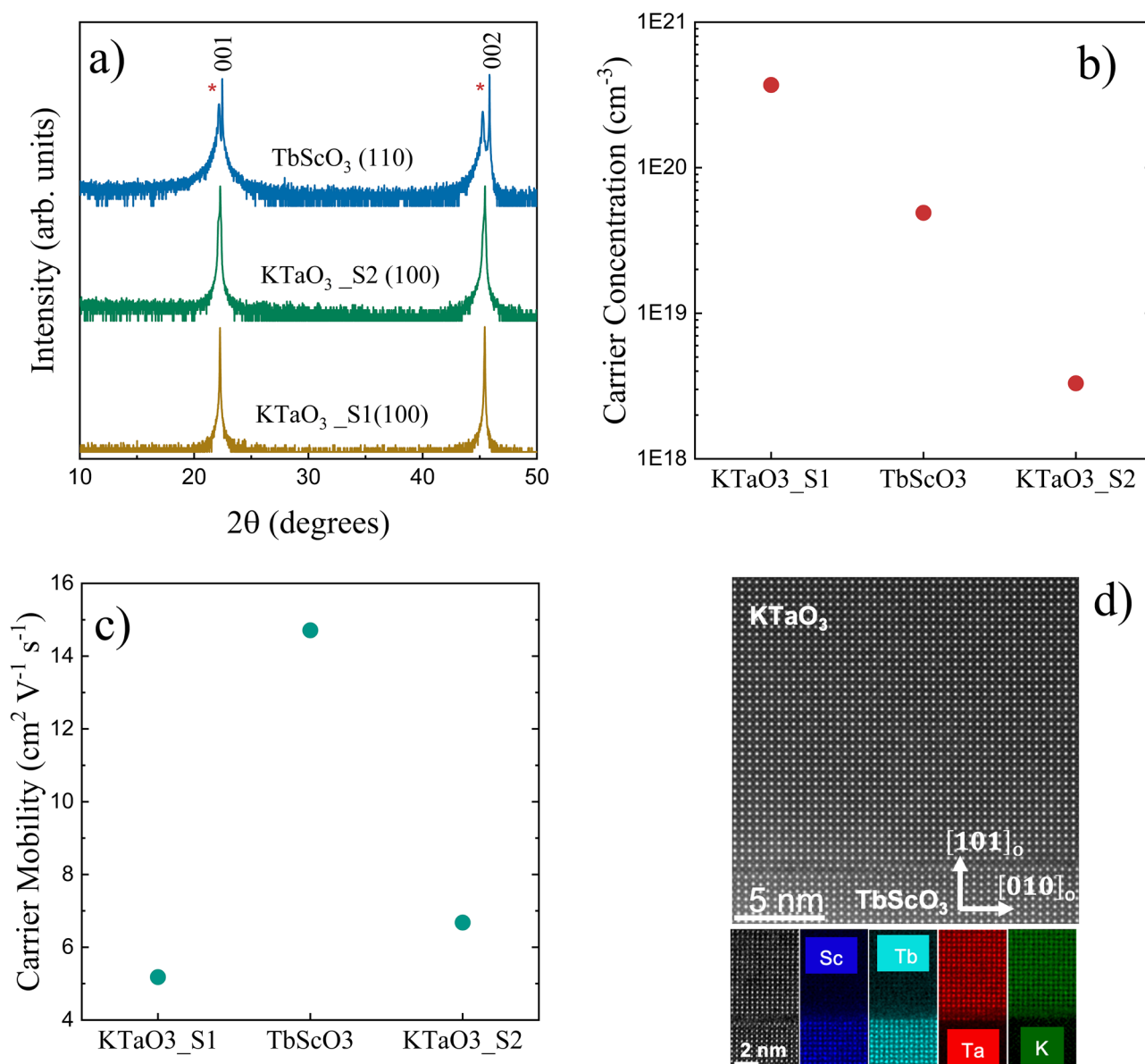


Fig. 2 | The thin films were characterized using X-ray diffraction (XRD), transport that ascertained the carrier concentration and mobility, and scanning transmission electron microscopy (STEM). a XRD measurement for the doped KTaO_3 thin film grown on two different substrates, KTaO_3 (100) and TbScO_3 (110)_o. XRD confirms that the samples are single phase and that the KTaO_3 films are aligned with the (100) plane parallel to the surface of the substrate. In the TbScO_3 (110)_o sample, we can clearly see the KTaO_3 thin film peaks aligning with the KTaO_3

substrate sample, along with the extra peaks from the TbScO_3 (110)_o substrate peaks. **b** Carrier concentration of the Ba-doped KTaO_3 thin film on both substrates at 100 K. The two samples grown on the KTaO_3 (100) substrate had $n = 3.7 \times 10^{20} \text{ cm}^{-3}$ and $3.3 \times 10^{18} \text{ cm}^{-3}$, while the one grown on TbScO_3 (110)_o had $n = 4.9 \times 10^{19} \text{ cm}^{-3}$. **c** Carrier mobility for all samples. **d** Scanning Transmission Electron Microscopy (STEM) of the grown KTaO_3 thin film on TbScO_3 (110)_o substrate.

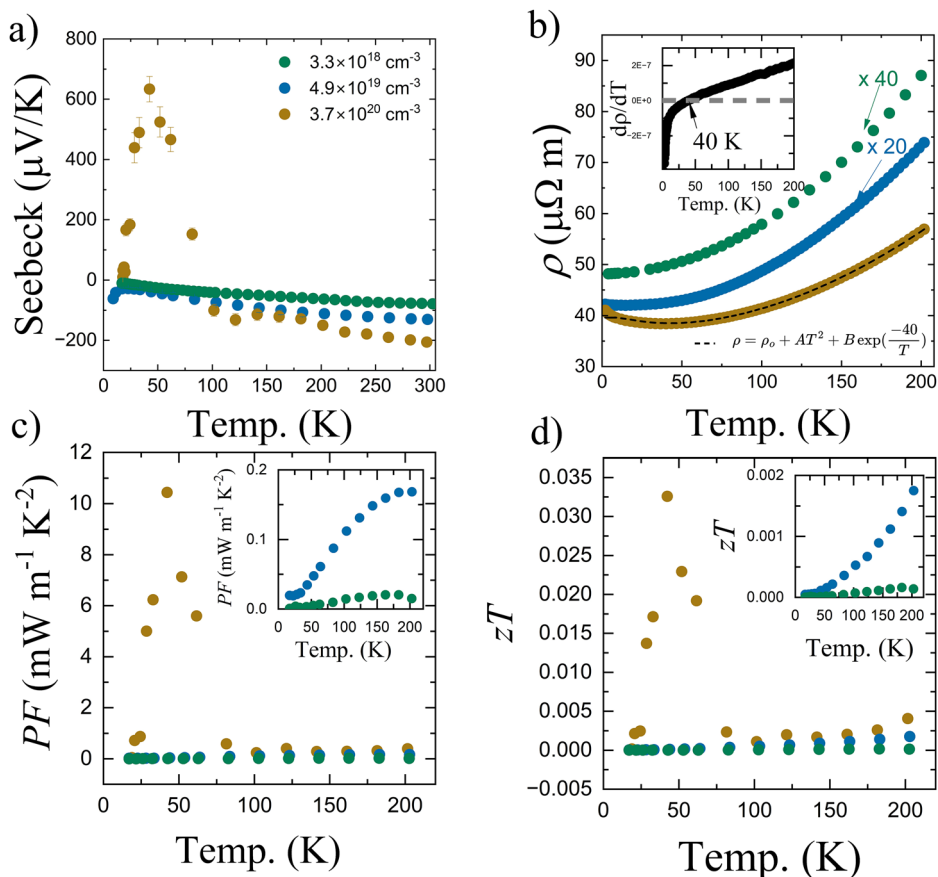
temperature¹⁰. Secondly, low defect concentration is needed to minimize phonon-defect scattering and increase the chance of electron-phonon scattering. In the case of our samples, we calculated the Fermi surface for all carrier concentrations using a tight-binding model fit from the *ab initio* band structure²⁸. In all cases, the Fermi surface has two bands, a uniform inner band, and a strongly warped outer band, shown in Fig. 1.

As illustrated in Fig. 1d, a minimum phonon wave vector ($\mathbf{q}_{\min}$) is required to satisfy the momentum conservation condition for the electron-phonon Umklapp process. To estimate its magnitude, we refer to the phonon band structure of KTaO_3 ²⁹, focusing on the longitudinal acoustic (LA) and transverse acoustic (TA) phonon modes. The LA mode reaches a maximum energy of 4 THz (~ 180 K), while the TA mode's maximum energy is at 2 THz (~ 90 K). For the higher carrier concentration sample, the minimum phonon wave vector required to meet the Umklapp

condition ($|\mathbf{k} + \mathbf{q}| > |\mathbf{g}|/2$), is estimated to be ~ 0.2 of the Brillouin zone (BZ). The corresponding phonon energies at this q -value are ~ 80 K for LA and ~ 40 K for TA modes. Both modes contribute to U-phonon-drag, but the TA mode is more populated at any temperature and U-phonon-phonon interactions limit the phonon-drag more at 80 K than at 40 K. Therefore, the TA mode is expected to contribute most, and the U-phonon-drag contribution to the Seebeck coefficient is expected to have a maximum near 40 K, as observed (Fig. 3a). Below this temperature, the number of phonons with that energy drops exponentially, causing the sharp decrease in Seebeck.

In contrast, the low carrier concentration sample, i.e., the sample with carrier concentration $4.9 \times 10^{19} \text{ cm}^{-3}$, requires a much larger minimum phonon wave vector (~ 0.8 BZ) to achieve Umklapp scattering. At this q -value, the phonon energies approach the Debye temperatures of the respective modes—approximately 180 K for LA and 90 K for TA. At these

Fig. 3 | The transport of all three samples was investigated, and their measured Seebeck and resistivity values, along with their calculated power factor (PF) and zT , were compared. a The thermopower measurements for the doped KTaO_3 thin films with three different carrier concentrations. The sample with the lowest carrier concentration ($3.3 \times 10^{18} \text{ cm}^{-3}$) displayed a negative linear thermopower down to 17 K. The sample with carrier concentration ($4.9 \times 10^{19} \text{ cm}^{-3}$) displayed a small negative phonon-drag effect at low temperature, illustrated by the downturn of the signal at the lowest temperatures. The behavior of the thin film with the higher carrier concentration ($3.7 \times 10^{20} \text{ cm}^{-3}$) is markedly different: the absolute value of the Seebeck signal linearly decreases until 100 K, the diffusive regime. Around 80 K, it changes sign. Then, it sharply increases until a peak occurs around 40 K. Afterwards, it sharply decreases as the temperature drops. Panel (b) displays the resistivity of the samples. The change in resistivity with respect to temperature (dp/dT) for the higher carrier concentration sample ($3.7 \times 10^{20} \text{ cm}^{-3}$) is shown in the inset. The minimum of resistivity and the peak in Seebeck drag align well around 40 K. The dashed curve through the data for that sample corresponds to an equation for the resistivity in the presence of Umklapp electron-phonon scattering. c, d Calculations of the power factor and thermoelectric figure of merit (zT); insets zoomed in to show the calculations for the samples with lower carrier densities.



higher energies, phonon-phonon U-scattering³⁰ overwhelms electron-phonon scattering.

Further, phonon-electron U-processes are resistive since the electrons undergo a Bragg reflection. U-phonon-drag is thus expected to induce an increase in electrical resistivity³¹. Such a change is clearly observed in Fig. 3b. At $T < 40$ K, where the Seebeck coefficient peaks, in the higher carrier sample, resistivity decreases with increasing temperature. This is contradictory to the behavior of normal metals and degenerately doped semiconductors, where resistivity increases with temperature, which is observed at $T > 40$ K. To further investigate this, we fit the data with the following function³¹:

$$\rho = \rho_0 + AT^2 + B \exp\left(\frac{-\Theta}{T}\right) \quad (3)$$

where the fitting parameters are set to $A = 5.3 \times 10^{-10} \text{ } \Omega \text{ m/K}^2$ and $B = 5.26 \times 10^{-6} \text{ } \Omega \text{ m}$. The second term of the equation (AT^2) represents the equilibrium electron-electron and electron-phonon scattering³², while the exponential term represents the U-phonon-drag scattering. Θ is the minimum temperature required for the phonon mode to satisfy the Umklapp scattering condition, i.e., the mode with $\mathbf{q}_{\min}$ in Fig. 1d and an energy of $\Theta = 40$ K as we previously determined. The addition of the Umklapp term in Eq. 3 gives the dashed curve in Fig. 3b; this explains very well the peculiar rise in resistivity below 40 K. The effect is absent in the low-doped samples. This is further evidence for electron-phonon Umklapp scattering in the highly doped sample.

Figure 3c, d show calculations of the power factor ($PF = \frac{S^2}{\rho}$) and thermoelectric figure of merit ($zT = \frac{S^2 T}{\rho \kappa}$). To calculate zT , we used the thermal conductivity of the KTaO_3 substrate because the thermal conductivity measurement was dominated by the substrate conductivity, and we cannot separate it from the thin film. The zT of the highest carrier

concentration sample reaches an astounding value of 0.032 at 40 K, which is about one order of magnitude higher than the lower carrier concentration sample. This highlights the important role of phonon-drag in enhancing the thermoelectric figure of merit in thin films.

Another detail to consider is the fact that Sakai et al. did not observe any phonon-drag or sign-change in their thermopower measurements on Ba-doped KTaO_3 ²⁷. These were bulk samples grown via the self-flux method and had carrier concentrations from mid- 10^{18} to low 10^{20} cm^{-3} . Additionally, the electrical resistivity of all their samples exhibited normal electron scattering that fitted a T^2 behavior ($\rho = \rho_0 + AT^2$). Our thin films had higher carrier concentrations than the bulk samples in the aforementioned study²⁷, and therefore a larger Fermi surface, enabling Umklapp scattering. Additionally, no phonon-drag was observed in all of the bulk-grown samples, indicating weak electron-phonon interaction²⁷.

A previous investigation into phonon-drag in thin films demonstrated that substrate acoustic phonons can propagate from the substrate into the thin films, where they interact with the charge carriers, thereby generating phonon-drag³³. The study reported that the phonon-drag contribution is generally less pronounced in bulk samples compared to thin films, which is consistent with our observations. Furthermore, it showed that the phonon-drag signal is influenced by the Debye temperature of the substrate. In our study, both KTaO_3 and TbScO_3 substrates have comparable Debye temperatures³⁰; hence, the interfaces are expected to be quite transparent to the acoustic phonons. Additionally, the sample with $3.3 \times 10^{18} \text{ cm}^{-3}$ carrier density, which was grown on KTaO_3 substrate, did not show the polarity reversal.

The above discussion is concerned solely with the acoustic phonon modes, as they typically have higher sound velocity and higher density of states compared to the optical modes. In the case of KTaO_3 , the lowest transverse optical mode (TO_1) exhibits a peculiar behavior; it has a relatively high sound velocity, comparable to that of the acoustic phonon mode,

enabling it to have a potential contribution to the thermal transport processes²⁹ at very high temperature. The TO₁ mode undergoes significant softening at the Γ point with decreasing temperature³⁴. At 100 K, the mode's energy is 78 K, which lies below the thermal energy of the system and is still populated, but exponentially less so than the TA phonons. As the temperature decreases to 40 K, the TO₁ mode softens further to an energy of 42 K. Even though the energy of the TO₁ mode at Γ is accessible in the range where thermopower changes sign, no softening has been confirmed at X, making the energy at higher k -points not accessible at low temperature. For Umklapp scattering, high k -vectors play a significant role. Therefore, acoustic phonons are more likely to be the main players in this scattering event.

In summary, we observed the reversal of phonon-drag thermopower polarity in Ba-doped KTaO₃ thin films mediated by electron-phonon Umklapp scattering. The polarity reversal occurs in a heavily doped sample (carrier concentration of $3.7 \times 10^{20} \text{ cm}^{-3}$) where the Fermi surface spans up to 0.8 of the Brillouin zone in some directions, enabling electron-phonon Umklapp scattering to occur, which reverses the electron momentum. This manifests as a positive thermopower below 80 K despite the n -type conduction, contrasting with conventional behavior in the lightly doped samples (3.3×10^{18} and $4.9 \times 10^{19} \text{ cm}^{-3}$) that maintained negative thermopower down to 2 K. The successful epitaxial growth of KTaO₃ films enables precise doping control, providing a platform to explore electron-phonon phenomena in quantum materials.

Methods

Material growth

Epitaxial thin films of KTaO₃ were grown using a modified Veeco Gen 10 MBE system, where the conventional SiC heater was replaced by 10 μm CO₂-laser from Epiray GmbH (THERMALAS Substrate heater). A molecular beam of TaO₂ (gas) flux was generated from an effusion cell containing Ta₂O₅ (H.C. Stark 99.99%) contained in an iridium crucible. TaO₂ is the most volatile species in the growth temperature range³⁵. Potassium was evaporated from an effusion cell containing an indium-rich (about 4:1 In:K ratio) mixture of potassium and indium, so it forms the air-stable intermetallic, In₄K. The K-In alloy was prepared in a glove box and contained in a titanium crucible. Once prepared, it can be exposed to air, facilitating its handling and loading. The vapor pressure of potassium is about 12 orders of magnitude higher than that of indium at the K-In cell temperature of 300–400 °C³⁶. TbScO₃ (110)o (Crytec GmbH) and KTaO₃ (MTI Corporation) substrates were used as received, where the O subscript indicates orthorhombic indices. Films were grown by co-deposition of potassium, TaO₂, and ozone, at substrate temperature of 900 °C as measured by an optical pyrometer operating at a wavelength of 7.5 μm . The films were grown at a background pressure of 1×10^{-6} Torr (10% O₃ and 90% O₂), and the K:Ta flux ratio was kept at approximately 10:1. A more detailed description is published elsewhere³⁷. Fluxes for the sources were $(3\text{--}4) \times 10^{13}$ atoms/cm²/s for TaO₂ and $(2\text{--}3) \times 10^{14}$ atoms/cm²/s for potassium, determined by a Quartz crystal microbalance (QCM). Barium fluxes were determined to be 1×10^{13} atoms/cm²/s at 500 °C and adjusted to doping concentrations with a calibrated vapor pressure curve³⁷. An accuracy of $\pm 15\%$ can be typically achieved by QCM flux calibration.

Transport measurements

Each sample was prepared for transport measurements by attaching the sample to a copper platform atop an alumina base acting as a heat sink. A strain gauge that supplied heat to the sample was adhered to the opposite side of the sample. Two type T thermocouples consisting of a copper and a Constantan wire were placed on one side of the sample to measure the temperature difference. The copper wires were used to measure the thermopower voltage (Fig. 1c). All parts were adhered using silver epoxy. The samples were then placed individually in a vacuum environment inside a Lakeshore helium-cooled cryostat. Current was supplied to the sample for electrical measurements and a strain gauge for thermal measurements via a 6221 Keithley current source. The voltages were read using a 2182 A Keithley

nanovoltmeter. The residual voltages were less than 2 μV , indicating great electrical contact. The cryostat temperature was controlled via a 331 Lakeshore temperature controller. The temperature was allowed to stabilize for 20 min before the sample heater was turned on. The temperature gradient was allowed to stabilize for 5 min before thermal measurements.

The value of the uncertainty on the Seebeck coefficient depends on both the noise level for the voltage and the temperature difference between the two thermocouples. The uncertainty on the 2182 A Keithley nanovoltmeter is 50 nV, and with a Seebeck value of 200 $\mu\text{V/K}$, it is negligible. The uncertainty of the temperature measurement on one thermocouple is 25 mK, so for the difference between two thermocouples, the uncertainty is 50 mK. We apply a temperature difference at room temperature of 3 K, making the uncertainty on the Seebeck coefficient at 300 K around 2%. At 100 K, the sensitivity of the type T thermocouple is lowered by one-half. Additionally, because the sample thermal conductivity increases and almost reaches its maximum value, the applied temperature gradient is lowered to about 1 K. This results in an uncertainty of about 10% below 100 K.

Data availability

The data that support the findings of this study are provided in the main text. Raw data related to the film growth and structural characterization in PARADIM facilities are available at <https://doi.org/10.34863/np1w-4394>. Additional raw data is available from the corresponding author upon reasonable request.

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Author contributions

B.L.W., K.A., and J.P.H. conceived the project; M.N., S.P., and B.L.W. performed thermoelectric and electric measurements, and analyzed the data with help from J.P.H and K.A.; S.P. and T.S. grew and characterized the samples with help from K.A. and D.G.S.; M.N.G. calculated the Fermi surface of the samples; S.S.R. conducted TEM; M.N., B.L.W., K.A., and J.P.H. wrote the manuscript with input from all coauthors. J.P.H. sadly passed away in the final stages of the review process.

Competing interests

The authors declare no competing interests.

Additional information

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