Correlated oxide Dirac semimetal in the extreme quantum limit

Jong Mok Ok1†‡, Narayan Mohanta1†, Jie Zhang1†, Sangmoon Yoon1, Satoshi Okamoto1, Eun Sang Choi2, Hua Zhou3, Megan Briggeman4,5, Patrick Irvin4,5, Andrew R. Lupini1, Yun-Yi Pai1, Elizabeth Skoropata1, Changhee Sohn1, Haoxiang Li1, Hu Miao1, Benjamin Lawrie1, Woo Seok Choi6, Gyula Eres1, Jeremy Levy4,5, Ho Nyung Lee1*  

Quantum materials (QMs) with strong correlation and nontrivial topology are indispensable to next-generation information and computing technologies. Exploitation of topological band structure is an ideal starting point to realize correlated topological QMs. Here, we report that strain-induced symmetry modification in correlated oxide SrNbO3 thin films creates an emerging topological band structure. Dirac electrons in strained SrNbO3 films reveal ultrahigh mobility ($\mu_{\text{max}} \approx 100,000 \text{ cm}^2/\text{Vs}$), exceptionally small effective mass ($m^* \sim 0.04m_e$), and nonzero Berry phase. Strained SrNbO3 films reach the extreme quantum limit, exhibiting a sign of fractional occupation of Landau levels and giant mass enhancement. Our results suggest that symmetry-modified SrNbO3 is a rare example of correlated oxide Dirac semimetals, in which strong correlation of Dirac electrons leads to the realization of a novel correlated topological QM.

INTRODUCTION

Gaining control over the properties of quantum correlation and topology in quantum materials (QMs) is a critical step in advancing the physics of QMs that can promote innovation in many technological areas (1–3), such as spintronics and quantum technologies. Therefore, the discovery of QMs in which both quantum correlation and topology are achieved is a subject of current interest. Quantum spin liquids (4–6), topological superconductors (7, 8), quantum anomalous Hall materials (9, 10), and fractional quantum Hall systems (11–16) are good examples of correlated topological QMs whose properties depend on both correlation and topology. Moreover, strongly correlated materials highlighting many-body interactions are good examples of material systems to study entanglement. Thus, creating and understanding entangled states in QMs are important steps toward quantum technologies. One way to achieve entangled states in solids is to reach the extreme quantum limit (XQL) (12, 15–17) (i.e., all carriers occupying entirely the lowest Landau level) at which correlations between charge carriers are maximized (18, 19). At the XQL, the strong correlation gives rise to fractional quasiparticles, and some of them are expected to obey nonabelian statistics (20, 21). The latter element is one of the most basic requirements for topological quantum computing.

Chalcogenide- and halogen-based materials have been at the center of the development of topological QMs (1–3, 22–24) because of their topological band structure and large spin–orbit coupling (SOC). However, the weak correlation in these topological materials hinders the appearance of key emergent phenomena, such as magnetism and superconductivity. Thus, the co-design approach, i.e., adding correlation to these topological materials, is currently under active investigation (22–24). A conventional approach includes both doping with 3d magnetic elements with strong correlation and creating heterostructures with magnetic and/or superconducting materials (7, 9, 10, 22–24). Such an approach, however, is a formidable task presenting a number of technical challenges.

In this context, transition metal oxides (TMOs) provide a versatile platform, owing to their inherent strong electron correlation and SOC (25, 26), as well as advancements in their thin-film synthesis and device fabrication. However, challenges also remain in studying TMOs, as the discovery of topological band structures is limited to only a couple of (or few) materials (27–30). Among oxide materials, 4d TMOs could be promising candidates, as they offer a good balance between electron correlation and SOC. Recently, a theoretical study predicted a topological band structure in an orthorhombic phase with $a^a \ c^c$ octahedral rotations in SrNbO3 (31). Dirac points in SrNbO3, however, were predicted to exist far from the Fermi level. Although the electronic structure of perovskite oxides can be modified through the strain control of octahedral rotations (32, 33), the viability of creating a novel Dirac semimetal with strained SrNbO3 by manipulating the octahedral rotations has not been explored.

RESULTS

To experimentally realize the Dirac semimetallic state theoretically predicted in the 4d perovskite SrNbO3 (31), an accurate determination of the crystallographic symmetry and its deliberate control are important. The utilization of epitaxial strain is known to be an effective method to modify the symmetry near the interface in a heterostructure (32, 33). Although the crystallographic details of the perovskite SrNbO3 have not been widely studied because of the difficulty of synthesizing the stoichiometric perovskite phase, a recent study with a polycrystalline perovskite SrNbO3, carried out through a lattice parameters of $a = 2a_p = 5.6894$ Å, $b = 2a_p = 5.6944$ Å, and $c = 2a_p = 8.0684$ Å ($\alpha = \beta = \gamma = 90^\circ$) with an orthorhombic structure (space group: $Pnma$) (34). With a pseudocubic approximation, the lattice parameter $a$ is

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1Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA. 2National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310, USA. 3Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439, USA. 4Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, USA. 5Pittsburgh Quantum Institute, Pittsburgh, PA 15260, USA. 6Department of Physics, Sungkyunkwan University, Suwon 16419, Korea.  
*Corresponding author. Email: hnlee@ornl.gov  
†These authors contributed equally to this work.  
‡Present address: Department of Physics, Pusan National University, Busan 46241, Korea.
4.023 Å (34, 35). In this work, we grew SrNbO₃ films on lattice-mismatched SrTiO₃ substrates [a₁ = 3.905 Å; therefore, the lattice mismatch of ε(%) = −3.02%] to induce epitaxial strain. To investigate the role of strain and the associated evolution of crystallographic symmetry, we systematically varied the thicknesses of films (d = 2.4 to 130 nm).

Epitaxial SrNbO₃ thin films were grown on (001) SrTiO₃ substrates by pulsed laser epitaxy. Despite the large lattice mismatch, high-quality SrNbO₃ thin films were successfully prepared, as was confirmed by several different methods, including reflection high-energy electron diffraction (RHEED), atomic force microscopy (AFM), x-ray diffraction (XRD), and cross-section scanning transmission electron microscopy (STEM) (see figs. S1 and S2). The films revealed sharp interfaces without any detectable interfacial mixing. In addition, the films were fully strained up to d₁ = 7 nm and partially strained from d₁ to d₂ = 18 nm. We observed that the NbO₆ octahedra were collectively distorted and rotated by the compressive strain. The fully strained film exhibited pronounced c° rotation-induced half-order peaks at (3/2 1/2 L/2), whereas these were absent in the fully relaxed thin films (Fig. 1C) (also see fig. S3). The relaxed films (d > d₂) exhibited a bulk-like cubic structure with an a°a°c° symmetry without any oxygen octahedral rotations (OORs; Fig. 1B). The octahedral distortions found in strained thin films significantly affected the electronic structure of this material. In the cubic SrNbO₃, there is no Dirac-like degeneracy (Fig. 1D), but the fourfold degeneracy remains intact at two high-symmetry points, P and N, in tetragonal SrNbO₃ with the a°a°c° symmetry. Nonsymmetric symmetry, i.e., screw rotation along the z direction, is known to protect the degeneracy at these two high-symmetrical points (see figs. S4 and S5) (36).

To investigate how epitaxial strain affects the transport properties of SrNbO₃ thin films, we first measured the temperature-dependent resistivity (T = 2 to 300 K) at different thicknesses and zero magnetic field (Fig. 2A). Our films (d = 2.4 to 27.2 nm) exhibit clear metallic behavior down to 2.4 nm in thickness. A gradual reduction in the overall resistivity is observed as the thin-film samples become partially strained at around the second critical thickness d₂ (Fig. 2B). In addition, the resistivity drastically increases at the ultrathin limit below d₁ (Fig. 2, A and B). The change in resistivity is attributed to a significant reduction in the carrier density (Fig. 2C and figs. S6 and S7), supporting a strain-induced electronic structure modification in SrNbO₃ ultrathin films, as expected from density functional theory (DFT) calculations. Note that such a huge change in carrier density is unusual, but it is reminiscent of topological materials, in which two to three order-of-magnitude changes in the carrier density have been reported when a transition from the topological phase to the correlated phase (e.g., superconductivity) occurred (37, 38). On the other hand, the resistivity of the relaxed films was around ~80 μΩ·cm at room temperature, which is of the same order of magnitude as a SrNbO₃ film grown on a KTaO₃ substrate with a smaller lattice mismatch (ε ~ −0.85%) (34). These results strongly suggest that the observed transport properties are intrinsic to SrNbO₃, ruling out a possible contribution from oxygen vacancies in SrTiO₃ substrates (see fig. S2).

Having established that transport behaviors were the intrinsic properties of SrNbO₃ thin films, we measured the Hall effect of our films with a wider range of film thickness (d = 2.4 to 74 nm) to further understand the strain effect on the electronic state. As shown in fig. S6, three different types of Hall effects are observed when the thickness is varied. Fully relaxed films (d > d₂) show a linear Hall effect, from which we extracted the carrier density (n = 1/|e|dB/dρₓₓ) and mobility (μ = (|e|ρₓₓn)⁻¹). The carrier densities of the relaxed films

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Fig. 1. Strain-induced Dirac metallic state in SrNbO₃ thin films. (A and B) Octahedral distortion pattern for (A) cubic SrNbO₃ (a°a°c° in the Glazer notation) and (B) strained tetragonal SrNbO₃ (a°a°c°). Epitaxial strain induces octahedral distortion. (C) Octahedral rotation-induced half-order superstructure diffraction peaks of (3/2 1/2 L/2) with L = 1, 3, 5 for fully strained (red, 7.2 nm, c° rotation) and fully relaxed (blue, 130 nm, c° rotation) SrNbO₃ thin films. r.l.u., reciprocal lattice unit. (D and E) Calculated electronic structure of (D) cubic SrNbO₃ and (E) strained tetragonal SrNbO₃. The red circle in plot (E) shows the Dirac point that appears near the Fermi level at the P point in the strained tetragonal phase. (F) Dirac dispersions near the P point within the tetragonal Brillouin zone. The larger Fermi velocity in the tetragonal phase, near the P point, would lead to higher carrier mobility and a favorable source of a nontrivial Berry phase in the presence of a magnetic field.
The values of the SrNbO$_3$/KTaO$_3$ samples mentioned previously \( \mu \approx 10,000 \text{ cm}^2/\text{V} \cdot \text{s} \) but extremely small carrier density. The mobility of the relaxed films was

\[
\mu_{\text{relaxed}} = \frac{1}{10,000 \text{ cm}^2/\text{V} \cdot \text{s}}
\]

and (D) mobility of SrNbO$_3$ thin films at 2 K. The carrier density of a relaxed thin film

\[
\rho = 2.4 \text{ to } 27.2 \text{ nm}
\]

Unlike the relaxed films, the strained samples \( \rho \approx 0.01 \text{ to } 0.02 \text{ cm}^{-3} \) exhibited non-

dependent Hall effects. The non-linear Hall effects can be explained by a two-carrier model by introducing an additional carrier (40), which presumably arises from the Dirac dispersion. The thickness-dependent carrier density and mobility are summarized in Fig. 2 (C and D). Note that the highest mobility observed is \( \mu_{\text{max}} \approx 100,000 \text{ cm}^2/\text{V} \cdot \text{s} \).

The additional small carriers evolve from holes into electrons as the thickness decreases.

To further investigate the quantum limit of a strained SrNbO$_3$ thin film \( (d = 6.4 \text{ nm}) \), we studied magnetotransport properties at 0.15 to 10 K up to 30 T. To check the reproducibility of our results, four different samples (named S1 to S4) were investigated (see fig. S8). All samples show clear quantum oscillations with qualitatively similar behaviors. First, we rotated the direction of the applied magnetic field with respect to the [001] axis and measured the quantum oscillations at several different angles \( (\theta = 0 \text{ to } 90^\circ) \) (Fig. 3A). The quantum oscillations become more apparent in their second derivatives \( (-d^2\rho/dH^2) \) (Fig. 3B). The quantum oscillations survive at higher angles and do not exhibit 1/cos\( \theta \) scaling; this behavior is attributed to the three-dimensional (3D) characteristics of the Fermi surface. The 3D character of the Fermi surface provides independent evidence to support the hypothesis that the transport properties originated from SrNbO$_3$ itself rather than from the interface with SrTiO$_3$ (see the Supplementary Materials for detailed discussions). The first evidence to support the quantum limit of SrNbO$_3$ thin films is an unsaturated linear magnetoresistance (MR) (Fig. 3C). At lower magnetic fields, the MR shows conventional \( H^0 \) behavior, but it changes to a linear MR at \( H^0_{\text{QL}} \approx 3.3 \text{ T} \) or higher. There are various possible mechanisms for this behavior. However, we attribute the unsaturated linear MR in the strained SrNbO$_3$ to quantum-linear MR (43) because it has a low carrier density. This unsaturated linear MR is a characteristic of Dirac/Weyl semimetals at the quantum limit, as has been reported for many Dirac/Weyl semimetals (44–46).

Another important piece of evidence of the quantum limit was found in quantum oscillations. Conventional quantum oscillations for higher Landau levels are periodic in inverse magnetic fields \( (1/H) \). However, the quantum oscillations recorded for strained SrNbO$_3$ films exhibit an intriguing aperiodic behavior (Fig. 4, A and B). This anomaly in the quantum oscillations provides an important characteristic unique to strained SrNbO$_3$ films. We attribute this quantum transport anomaly to the fractional occupation of the Landau levels owing to the strong correlation. As illustrated in fig. S9, we found that the Landau fan diagram \( (1/H \text{ versus } N) \) deviates significantly from the linear dependence when it is plotted by assigning the minima of resistivity—i.e., the second derivative of \( \rho_{xx} \) in a SrNbO$_3$ thin film is considered, the minima of \( \rho_{xx} \) can be assigned to \( N \) because \( \sigma_{xx} = \rho_{xx}/(\rho_{xx}^2 + \rho_{xy}^2) \approx A\rho_{xx} \), where \( A \) is a prefactor. Such a strong deviation is obviously different from conventional quantum oscillations, even considering Zeeman splitting. On the other hand, the Landau fan diagram exhibits a clear linear relationship when the minima of the quantum oscillations are assigned to the rational fractions of the Landau integers \( N = 1/3, 2/3, 4/3, 5/3, 2/5, 3/5, 4/5, 5/5, 3/7, 4/7, 5/7, 6/7, \) and 4/9 (Fig. 4, A and B) (also see fig. S9). To ensure the reproducibility of this intriguing phenomenon, we tested four different samples, and it was observed consistently in all the samples (see Fig. 4C and figs. S8 and S9). We further note that while the origin is still under debate, similar aperiodic quantum oscillations were reported in the 3D topological semimetal ZrTe$_5$ (16, 17).

**DISCUSSION**

The entire series of fractional numbers of Landau integers seen in our strained perovskite oxide is highly extraordinary, as only extremely clean systems, including graphene (11) and GaAs-based 2D electron gases (2DEGs) (12), have revealed such a complete set of fractional states. Only a portion of the fractional numbers have been

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**Fig. 2. Thickness dependence of electronic state of SrNbO$_3$ thin film.** (A) Temperature dependence of resistivity of SrNbO$_3$ thin films with various thicknesses of 2.4 to 27.2 nm. (B to D) Thickness dependence of (B) resistivity, (C) carrier density, and (D) mobility of SrNbO$_3$ thin films at 2 K. The carrier density of a relaxed thin film is well explained by the \( d^2 \) electron configuration. An additional electron carrier, which has high mobility \( \mu = 10,000 \text{ cm}^2/\text{V} \cdot \text{s} \) but extremely small carrier density \( n = 1.5 \times 10^{18} \text{ cm}^{-3} \), is observed in the strained thin films. The additional electron band has an experimentally reachable quantum limit of \( H^0_{\text{QL}} \approx 3.3 \text{ T} \) because of its extremely small carrier density.
Fig. 3. Angular dependence of quantum oscillations. (A) MR for different angles up to 30 T at 0.3 K. Inset shows MR for different temperatures (T=0.15 to 10 K). Quantum oscillations and linear MR are clearly observed in SrNbO₃. (B) Second derivative of resistivity (−d²ρ/dH²) for different angles. Quantum oscillations are observed for all different angles and do not follow the 1/5θ behavior, supporting the 3D character of the Fermi surface. (C) First derivative of resistivity (dρ/dH) for two different samples at 0.3 K. The linear MR starts to develop at H*QL ~ 3.3 T.

observed in previously reported 2D systems at the quantum limit, such as a silicon quantum well (13), MnZnO/ZnO (14), and the surface state of Bi₂Se₃ (15), MnZnO/ZnO (14), such as a silicon quantum well (13), and ZrTe (16), and ZrSIs (50), those systems showed only a miniscule increase in effective mass of up to ~300%.

Overall, these findings indicate that symmetry-modified SrNbO₃ is a 3D correlated oxide Dirac semimetal entering the XQL, in which topology meets many-body physics, yielding fractional occupation of Landau levels. Thus, we think that SrNbO₃ offers a promising platform for further exploration of exotic correlated quantum phases and behaviors that can provide innovative materials solutions for the next generation of quantum technologies.

MATERIALS AND METHODS
Film growth
Substrates of TiO₂-terminated SrTiO₃ (001) 5 × 5 mm² in size were prepared by etching with buffered hydrofluoric acid and annealing at 1000°C for 1 hour. A ceramic target was prepared by sintering mixtures of stoichiometric amounts of SrCO₃ and Nb₂O₃ powder at
1100°C for 10 hours, with an intermediate grinding and pelleting step after the initial decarbonation step at 1000°C for 12 hours. A KrF excimer laser (λ = 248 nm) was used to ablate the target at a repetition rate of 5 Hz. SrNbO₃ thin films were grown on SrTiO₃ (001) substrates at optimum conditions of Tₐ = 650°C, PO₂ < 4 × 10⁻⁶ torr, and f = 0.4 J/cm². Owing to the 5+ preference of the niobium valence, the perovskite phase (Nb⁴⁺) is achieved only under precisely controlled conditions of oxygen pressure (PO₂ < 10⁻⁵ torr) (34, 35), similar to the conditions needed for LaTiO₃ (51, 52).

Film thickness was calibrated by x-ray reflectivity using a four-circle diffractometer. Crystallinity and epitaxial strain were examined by XRD and reciprocal space mapping. The surface morphology measurements were made with an AFM (Veeco Dimension 3100). Figure S1A shows XRD patterns of the SrNbO₃ 002 peak at different thicknesses (d = 2.4 to 15.2 nm). We observed a clear peak position shift at the critical thickness of d₁ = 7 nm, which is consistent with the huge jump in low-temperature resistivity (see Fig. 2, A and B). Our thin films had atomically flat surfaces, as confirmed by the AFM image and the RHEED image shown in fig. S1 (B and C, respectively).

**Charge accumulation at the interface from STEM-EELS analysis**

Cross-sectional TEM specimens were prepared using low-energy ion milling at LN₂ temperature after mechanical polishing. High-angle annular dark field (HAADF) STEM measurements were performed on a Nion UltraSTEM200 microscope operated at 200 kV. The microscope was equipped with a cold field-emission gun and a corrector of third- and fifth-order aberrations for sub-angstrom resolution. A convergence half-angle of 30 mrad was used, and the collection inner and outer half-angles for HAADF STEM were 65 and 240 mrad, respectively. A collection aperture of 5 mm was used for electron energy loss spectroscopy (EELS) measurement, and EELS spectrum imaging was performed at a speed of 30 frames per second.

Figure S2A shows HAADF STEM image of a SrNbO₃(d = 6.5 nm)/SrTiO₃ sample viewed along the [100] zone axis. The HAADF STEM image confirms that the SrNbO₃ thin film is epitaxially grown on the SrTiO₃ substrate with a sharp interface. Note that the nonuniform background contrast in the HAADF STEM image can be attributed to the amorphized surface of the TEM specimen, which was formed by argon ion milling. Figure S2 (B and C) shows the integrated Ti-L₂,₃ and O-K edge EELS spectra across the interface. As shown in fig. S2B, the spectral features of the Ti-L₂,₃ edge broaden with the approach from the substrate to the interface. Note that the spectral change is most prominent at the first unit cell of the substrate, and the EELS spectrum fully returns to the spectrum of standard SrTiO₃ from three unit cells below. This spectral change is attributed to the charge transfer from the SrNbO₃ thin film.

The broadening of the Ti-L₂,₃ edge spectra in SrTiO₃ could be due to any of the following three reasons (53): symmetry change at the interface, charge reduction due to oxygen vacancies, or charge reduction due to charge transfer from heteromaterials. On the basis of the HAADF STEM image, the first possibility can be ruled out because a sharp interface with a robust epitaxial relationship is observed. To further examine the origin of the charge reduction, we estimated the ratio between the titanium and oxygen continuum parts from the substrate bulk to the interface (fig. S2D). The continuum parts were used for the stoichiometry analysis because the near-edge structure was sensitive to the internal electronic states. As shown in fig. S2D, there was no significant difference between the interface and the substrate bulk. Rather, the ratio became higher at the interface layer of SrTiO₃, which can be attributed to the beam broadening (the signals from SrNbO₃ can additionally contribute to the O-K edge). The stoichiometry analysis suggested that the spectral change at the interface (1 unit cell of SrTiO₃) was mainly due to the charge transfer from the SrNbO₃ thin film.

In addition to the EELS results, there are several other pieces of evidence that the charge transfer from the SrNbO₃ thin film, not oxygen vacancies, induced the charge accumulation at the interface. During pulsed laser deposition, vacancies can be formed when high-energy plasma plumes collide with the substrate. Therefore, the formation of oxygen vacancies depends to a great extent on the growth conditions, mainly the oxygen pressure and laser fluence. Higher vacuum and laser fluence create more oxygen vacancies. Oxygen stoichiometric films, however, can be grown even in a high vacuum if the laser spot size and energy are optimized, as our group reported earlier (54). We used a laser with a low enough fluence (f = 0.4 J/cm²) to grow SrNbO₃ thin films. To check for a possible oxygen deficiency in the substrate, we grew SrTiO₃ film on a SrTiO₃ substrate in the same growth conditions used for the SrNbO₃ thin films. The SrTiO₃ thin films that were grown were totally insulating, supporting the hypothesis that interfacial charges are not related to oxygen deficiency. Thus, charge transfer was most likely the origin of interfacial electrons, as predicted by a theoretical study (55). Unlike oxygen vacancies, which can extend deep into the SrTiO₃ side (56), charge transfer is expected only at the interface (57) (maximum of 2 to 3 unit cells of SrTiO₃), which matches our observations well.

**Lattice symmetry and strain-induced octahedral rotation of SrNbO₃**

As shown in fig. S3 (A and B), we used x-ray Bragg rod diffraction L scans at four different H-K quadrants to check and determine the primary lattice symmetry of SrNbO₃ as a function of film thickness. We present the fully strained 7.2-nm and fully relaxed 130-nm films as representative results (we also similarly measured 1.8-, 16-, and 20-nm SrNbO₃ films). Both strained and relaxed SrNbO₃ films displayed fourfold rotational symmetry. The 7.2-nm film showed a tetragonal-like lattice symmetry (c ≈ a) as a result of the compressive strain, whereas the 130-nm film revealed a cubic-like lattice symmetry (c = a). OOR-induced perovskite lattice doubling produced a unique set of half-order superstructure Bragg peaks, which were used to determine the OOR pattern and quantify the rotation angles. For detailed OOR half-order peak investigations with very weak signals, we carried out synchrotron XRD measurements at room temperature at beamline 33-ID-D at the Advanced Photon Source at Argonne National Laboratory. Monochromatized x-rays with a wavelength of 0.61992 Å were used, and a Pilatus 100K photon-counting area detector was used to capture the weak half-order superstructure. To suppress the fluorescence signal of the SrTiO₃ substrate, higher-energy x-rays (E = 20 keV, well above the Sr K absorption edge) were chosen. Scattering geometric corrections and background subtractions using a photon-counting area detector were conducted for all films. We surveyed all possible types of OOR half-order peaks to determine the rotation pattern with Glazer notation. The total absence of (odd/2, even/2, odd/2), (odd/2, odd/2, even/2), and (odd/2, even/2, even/2) types of peaks ruled out the existence of in-phase (+) rotation along either the a or c lattice axis or the existence of perovskite A-site cation off-symmetry point displacement (not shown in fig. S3). As shown in fig. S3C, the (H/2 K/2 L/2) (H = K) type peaks are also
experimental lattice constants $a = 5.518$ Å, found to be sufficient to achieve convergence of the total energy.

The calculated Fermi surfaces of SrNbO$_3$ in the cubic (relaxed) and the tetragonal (strained) phases are shown in fig. S4. The three Fermi surfaces correspond to the three t$_{2g}$ orbitals of niobium. The calculated band structure and Fermi surfaces of the cubic SrNbO$_3$ are consistent with recent reports (60, 61). The heavier electronic band constitutes a larger Fermi surface in both the cubic and tetragonal phases. The Dirac point at the P point near the Fermi level in the tetragonal phase is visible in the Fermi surface (bottom left plot) in the form of a connection between two disjoint surfaces (small surface with blue top and bigger surface with yellow top) at the P point.

Because the Dirac point at the P point is closer to the Fermi level, it can act as a source of a nontrivial Berry phase in the presence of a magnetic field. On the other hand, the Dirac points at the N point appear at $-0.7$ eV above the Fermi level. Although these Dirac points at the N point are energetically unfavorable, oxide heterostructures would offer an avenue for designing a Dirac metallic phase by tuning the Fermi level closer to these Dirac points by strain or chemical substitution.

The Fermi velocity and effective mass near the Dirac point were estimated to be $7.07 \times 10^5$ m/s and 0.026 m$_e$, respectively. The high Fermi velocity near the P point was also expected to give rise to a high carrier mobility in strained SrNbO$_3$ thin films.

**Band structure calculation**

First-principles electronic structure calculations were carried out within the framework of DFT on a plane wave basis with Perdew-Burke-Ernzerhof (PBE) exchange correlation (58), as implemented in the QUANTUM ESPRESSO simulation code (version 6.5) (59). We used a $7 \times 7 \times 8$ Monkhorst-Pack $k$-point mesh to discretize the first Brillouin zone and a plane wave cutoff of 600 eV, which were found to be sufficient to achieve convergence of the total energy. The energy convergence criterion was set to $10^{-6}$ eV during the minimization process of the self-consistent cycle. More detailed information regarding the strain, symmetry, and octahedral rotation of SrNbO$_3$ thin films with different thicknesses is summarized in table S1. Both $\gamma$ angles for 7.2- and 16-nm strained films are close to 10$^\circ$, which was used for the DFT calculations. The ultrathin 1.8-nm film exhibits a relatively reduced $\gamma$ angle, probably because of the proximity effect of octahedral connectivity imposed by the underlying SrTiO$_3$ substrate without any OOR ($a^0 a^0 a^0$).

**Strain-tunable Dirac metallic state in SrNbO$_3$**

As observed in our lattice symmetry measurements and octahedral rotation-induced half-order superstructure diffraction measurements, the substrate strain in the thin-film limit stabilized SrNbO$_3$ into a tetragonal crystalline symmetry (space group: $I4/mcm$) in which the NbO$_6$ octahedra were rotated only in the $x$-y plane along the z axis. As discussed in the main text, Dirac points appeared at the P point and at the N point of the Brillouin zone in this tetragonal crystalline environment. Figure S5 shows the band dispersions at three different levels of the octahedral rotation. The Dirac point at the P point is found to remain closer to the Fermi energy in all three cases. The three Dirac points at the N point come closer to the Fermi energy with increasing octahedral rotation, as shown in fig. S5 (D to F), enabling them to be available in the electronic transport. The octahedral rotation, therefore, offers a route to tune the Dirac points in a controlled manner that can be efficiently engineered in oxide heterostructures by using the substrate strain.

**Transport measurements**

Electrical transport measurements in this work were conducted with three measurement systems: the 14 T Physical Property Measurement System (Quantum Design), an 18 T dilution refrigerator at the University of Pittsburgh, and a 30 T bitter magnet with a He$^3$ cryostat at the National High Magnetic Field Laboratory (Tallahassee, USA). Results from different systems and different samples were reproducible and consistent. Aluminum wire-bonded contacts with a Van de Pauw configuration were used for measuring magnetotransport properties.

**Strain-tunable multiband nature of SrNbO$_3$ thin films**

Figure S6A shows the normalized Hall resistivity $\rho_{xy}$ of SrNbO$_3$ thin films with different thicknesses. Although a fully relaxed thin film ($d = 74$ nm) shows linear Hall effects, nonlinear Hall effects were observed in the strained films ($d < d_c$). To explain the observed nonlinear Hall effects in the SrNbO$_3$ thin films, a semiclassical two-band model was used

$$\rho_{xy} = \frac{(\mu_e^2 n_h + \mu_h^2 n_e)}{e (|\mu_e| + |\mu_h|)} + B (n_e + n_h)$$

with the restriction of zero field resistivity

$$\rho_{xx}(0) = \frac{1}{e (|\mu_e| + |\mu_h|)}$$

where $n_e$ ($n_h$) and $\mu_e$ ($\mu_h$) are the carrier density and mobility, respectively, for electron(hole) type charge carriers. Figure S6B shows the magnetic field dependence of $\rho_{xy}$ ($H$) (black dots) with fitting curves (colored solid lines). The convex-shaped $\rho_{xy}$ ($H$) for a 6.4-nm thickness film was well explained by using two electron carriers, and the concave-shaped $\rho_{xy}$ ($H$) found in the 12.4-nm-thickness film was captured by electron and hole carriers.

Figure S7 shows the temperature dependence of the estimated mobility and carrier density for strained ($d = 6.4$ nm) and fully relaxed ($d = 74$ nm) SrNbO$_3$ thin films. The temperature dependence of the electron mobility for both samples shows typical behavior, which follows the Matthiessen rule: $\mu^{-1} = \mu_0^{-1} + \mu_{c,sp}^{-1} + \mu_{c,OP}^{-1}$, where $\mu_0$ describes the temperature-independent scattering from impurities or interface roughness that dominates at low temperature, $\mu_{c,sp} \propto T^2$ quantifies the electron-electron scattering for intermediate temperatures,
and \( \mu_{\text{iO}} \) is the high temperature-dependent electron-phonon scattering term (62). The carrier densities of two different samples, however, show clearly different degrees of temperature dependence. Whereas the carrier density of the relaxed film does not change significantly, that of the strained film decreases by two orders of magnitude at low temperature. These observations further highlight the strain-induced electronic structure change. As explained earlier, two types of electrons contribute to the transport properties of the strained thin film: one with high mobility and low carrier density, and the other with low mobility and high carrier density. The former can be regarded as the origin of the quantum oscillation with the Dirac nature, as discussed in detail in the main text. The latter, however, may come from a simple parabolic band and may not be able to generate quantum oscillations because of a large scattering rate. Under such a multicarrier condition, the longitudinal and Hall conductivities can change as a function of magnetic field. Under such a condition, the effective mass does not change as a function of magnetic field. However, the strong magnetic field dependence of the effective mass is clearly seen in strained SrNbO\(_3\) films. The magnetic field dependence of the effective mass is summarized in Fig. 4.

### Aperiodic oscillations

Figure S8 (A and B) displays the low-temperature MR and Hall resistivity of different SrNbO\(_3\) thin films with almost the same thickness, \( \sim 6.4 \) nm. All samples (S1 to S4) show consistent oscillations and the convex-shaped Hall effect that can be explained by the presence of two electron carriers, as previously discussed. Note that the oscillations are seen only in the films that have convex-shaped Hall effects. This finding supports the idea that one of the electron carriers, with low carrier density and high mobility, contributes to the oscillations. The oscillations are more pronounced in the second derivative curves \((-d^2p/dH^2)\), as shown in fig. S8C. The minima of resistance are consistent with the minima of the second derivative, as displayed in fig. S9A.

By assigning the minima in oscillations to an integer Landau level index \( N \), we plotted the Landau fan diagram as illustrated in fig. S9C. The \( 1/H \) versus \( N \) deviates significantly from a conventional linear dependence. This unusual behavior cannot be explained even considering the strong Zeeman splitting with an enormous Lande g-factor. For the unconventional behavior to be explained as the effect of Zeeman splitting, at least the low–magnetic field region would have to show linear behavior, and its extrapolated line should be passing through near \( N = 0 \). However, we could not find any field region in which the Landau fan diagram showed linear behavior, even under a low magnetic field. Furthermore, the slope of the Landau fan diagram in a low–magnetic field region is too steep to pass \( N = 0 \). The deviation from conventional linear dependence is observed even in the low–magnetic field \( H < 3 \) T, at which the Zeeman effects are negligible (Zeeman energy \( \sim 0.5\) meV). The unusual periodicity of oscillations, however, can be understood if the fractional Landau levels are taken into account, as discussed in the main text.

Note that aperiodic oscillations were also reported in LaAlO\(_3/\)SrTiO\(_3\) samples. They were attributed to apparent spin degeneracy (65) and magnetic field–dependent electronic bands of titanium \( d_{xy}/d_{xz} \) orbitals (66). Both cases were based on the large effective mass of 1.4 to 1.7 \( m_e \) as experimentally confirmed. Unlike the behaviors of LaAlO\(_3/\)SrTiO\(_3\) 2DEGs, the SrNbO\(_3\) films had an extremely small effective mass and giant mass enhancement at high fields that cannot be explained by the scenarios used for LaAlO\(_3/\)SrTiO\(_3\).

### Strong mass enhancement at quantum limit

Figure S10 illustrates the magnetic field dependence of oscillations at different temperatures, showing their clear temperature and field dependence. With the temperature dependence of oscillations, the effective mass \( m^* \) can be estimated by using the Lifshitz-Kosevich formula \( \Delta \rho_{\text{xx}} \sim (\alpha m^* T/H) \sinh(\alpha m^* T/H) \), where \( \alpha = 2\pi c k_B \approx 14.69\) T/K. Figure S10A shows mass plots for oscillations under several magnetic fields. In conventional cases, the effective mass does not change as a function of magnetic field. However, the strong magnetic field dependence of the effective mass is clearly seen in strained SrNbO\(_3\) films. The magnetic field dependence of the effective mass is summarized in Fig. 4.

### Origin of transport properties

Although there was charge accumulation at the interface, the transport properties were dominated by the SrNbO\(_3\) rather than by the interface. Figure S11 shows the carrier density dependence of mobility for the SrNbO\(_3/\)SrTiO\(_3\) thin films and SrTiO\(_3\)-related materials (67). SrNbO\(_3\) itself is the metal, with a huge number of carriers, \( n \approx 10^{21} \) cm\(^{-3}\), which is three to five orders of magnitude larger than the number in the 2DEG in SrTiO\(_3\)-related materials. Furthermore, the carriers with a larger density, \( n \approx 10^{21} \) to \( 10^{22} \) cm\(^{-3}\), in SrNbO\(_3\) show one order of magnitude higher mobility than the 2DEG. The difference results from the effective mass difference between the two materials (\( m^* \approx 0.1\) \( m_e \) for SrNbO\(_3\) and \( m^* \approx 1\) to 2 \( m_e \) for 2DEG in SrTiO\(_3\)). The transport properties observed in SrNbO\(_3/\)SrTiO\(_3\), therefore, originated from the SrNbO\(_3\) itself rather than from the interface, because of the larger carrier density and higher mobility of SrNbO\(_3\).

In addition, the observed quantum oscillations were not related to the interfacial electrons for the following reasons. First, the effective mass estimated from quantum oscillation is too light to be explained with a 2DEG. The typical effective mass of a SrTiO\(_3\)-based 2DEG is \( \sim 1 \) to \( 2\) \( m_e \) as found in LaAlO\(_3/\)SrTiO\(_3\) (68), Al\(_2\)O\(_3/\)SrTiO\(_3\) (69), and so on. Second, the quantum oscillation captures the 3D feature of the Fermi surface. The EELS spectrum directly verified that the excess electrons were mostly localized at the first monolayer of the substrate, which cannot account for the 3D Fermi surface. The 3D character can arise if the electron wavelength is smaller than the thickness. On the basis of the de Broglie relation, the electron wavelength is \( \lambda = h/(m^* v) \). For a typical 2DEG in SrTiO\(_3\), the wavelength is estimated to be \( \sim 0.7 \) nm (\( v = 10^6 \) m/s and \( m^* = 1\) \( m_e \) for typical electrons). Thus, 1- to 2-unit cells of SrTiO\(_3\) exhibit a 2D character (\( \lambda \gg d \)) as previously reported (68). On the other hand, metallic SrNbO\(_3\) can have a 3D Fermi surface. By considering the Fermi velocity of SrNbO\(_3\) near the Dirac point \( v = 7.07 \times 10^7 \) m/s, which is an order of magnitude higher than the typical electron velocity of \( 10^6 \) m/s, one can estimate the wavelengths of SrNbO\(_3\) electrons. The wavelength of SrNbO\(_3\) at a low field with \( m^* \approx 0.1\) \( m_e \) is expected to be \( 0.1 \) nm (\( \lambda \ll \) thickness); thus, SrNbO\(_3\) could give rise to a 3D feature.

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**SUPPLEMENTARY MATERIALS**

Supplementary material for this article is available at https://science.org/doi/10.1126/sciadv.abf9631
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Acknowledgments: We thank J. S. Kim, Y. Kim, and M. Brahelek for discussion. Funding: This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, and in part by the Computational Materials Sciences Program. The high–magnetic field measurements were performed at the National High Magnetic Field Laboratory, which is supported by NSF cooperative agreement no. DMR-1644779 and the state of Florida. This research used resources of the Advanced Photon Source, a DOE Office of Science User Facility, operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02-06CH11357. Extraordinary facility operations were supported, in part, by the DOE Office of Science through the National Virtual Biotechnology Laboratory, a consortium of DOE national laboratories focused on the response to COVID-19, with funding provided by the Coronavirus CARES Act. W.S.C. was supported by Basic Science Research Programs through the National Research Foundation of Korea (NRF) (NRF-2021R1A2C2011340). J.L. acknowledges support from NSF (PHY-1913034) and Vannevar Bush Faculty Fellowship (N00014-15-1-2847). Author contributions: J.M.O. and H.N.L. conceived the project. J.M.O. and J.Z. grew films and conducted characterization with help from E.S., C.S., H.L., H.M., W.S.C., and G.E. N.M. and S.O. performed DFT calculations. S.Y. and A.R.L. conducted STEM experiments. H.Z. conducted synchrotron XRD measurements. J.M.O. performed transport measurements with help from J.Z., E.S.C., Y.-Y.P., B.L., M.B., P.L., and J.L. J.M.O. and H.N.L. wrote the manuscript with input from all authors. Competing interests: The authors declare that they have no competing interests. Data and materials availability: All data needed to evaluate the conclusions in the paper are presented in the paper and/or the Supplementary Materials.

Submitted 1 December 2020 Accepted 23 July 2021 Published 15 September 2021 10.1126/sciadv.abf9631

Citation: J. M. Ok, N. Mohanta, J. Zhang, S. Yoon, S. Okamoto, E. S. Choi, H. Zhou, M. Briggeman, P. Irvin, A. R. Lupini, Y.-Y. Pai, E. Skoropata, C. Sohn, H. Li, H. Miao, B. Lawrie, W. S. Choi, G. Eres, J. Levy, H. N. Lee, Correlated oxide Dirac semimetal in the extreme quantum limit. Sci. Adv. 7, eabf9631 (2021).