

RAPID COMMUNICATION

Room-temperature bulk plasticity and tunable dislocation densities in KTaO_3 Xufei Fang^{1,a,#} | Jiawen Zhang^{2,#} | Alexander Frisch^{1,a} | Oliver Preuß³ |
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Editor's Choice

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Abstract

We report room-temperature bulk plasticity mediated by dislocations in single-crystal cubic potassium tantalate oxide (KTaO_3), contrasting the conventional knowledge that single-crystal KTaO_3 is susceptible to brittle fracture. A mechanics-based combinatorial experimental approach using cyclic Brinell indentation, scratching, and uniaxial bulk compression consistently demonstrates room-temperature dislocation plasticity in KTaO_3 from the mesoscale to the macroscale. This approach also delivers tunable dislocation densities and plastic zone size. Scanning transmission electron microscopy analysis underpins the activated slip system to be $\langle 110 \rangle \{1\bar{1}0\}$. Given the growing significance of KTaO_3 as an emerging electronic oxide and the increasing interest in dislocations for tuning the physical properties of oxides, our findings are expected to trigger synergistic research interest in KTaO_3 with tunable dislocation densities.

KEYWORDS

bulk compression, cyclic deformation, dislocation, KTaO_3 , scanning transmission electron microscopy[#]These authors contribute equally to this work.^aPreviously in the Department of Materials and Earth Sciences at the Technical University of Darmstadt where this work was initiated.This is an open access article under the terms of the [Creative Commons Attribution](https://creativecommons.org/licenses/by/4.0/) License, which permits use, distribution and reproduction in any medium, provided the original work is properly cited.© 2024 The Author(s). *Journal of the American Ceramic Society* published by Wiley Periodicals LLC on behalf of American Ceramic Society.

1 | INTRODUCTION

Ceramics are generally known for their brittleness at room temperature, primarily due to the lack of dislocation-mediated plasticity. Recent advancements have demonstrated room-temperature dislocation plasticity in various ceramic materials at small scales using techniques like nanoindentation^{1–3} and nano-/micropillar compression.^{4,5} These methods minimize flaw populations and favor plastic flow over cracking or suppress crack propagation through locally high compressive hydrostatic stress (as seen in nanoindentation with shallow depth) or by reducing the deformed volumes (in nano-/micropillar compression).

In contrast, ceramics that exhibit bulk and mesoscale plasticity under ambient conditions are relatively rare, despite their long research history. Alkali halide crystals, such as LiF, NaCl, and KCl, have been extensively studied for their dislocation mechanics since the 1950s. Classic studies by Johnston and Gilman on LiF single crystals have systematically explored dislocation multiplication, nucleation, and mobility through dislocation etch pit studies.^{6–8} Similarly, NaCl crystals have been pivotal in understanding dislocation-based fracture toughness^{9,10} and electro-plasticity as well as the charge of dislocations in ionic crystals.¹¹ Another notable group of ductile ceramics includes simple oxides with rock-salt structures, for instance, single-crystal MgO. Discovered to be plastically deformable in bulk compression^{12,13} as early as in the late 1950s, MgO continues to be studied for its fundamental role in the Earth's lower mantle¹⁴ and as a model system for understanding the elementary dislocation mechanics in oxides.¹⁵

Due to the wide bandgap of the aforementioned ductile crystals, their application in electronic devices is limited. Consequently, more attention has been directed towards other ductile semiconductors such as ZnS¹⁶ and perovskite oxides. In 2001, Brunner et al.¹⁷ reported the *surprising* discovery of room-temperature plasticity in SrTiO₃ (cubic structure) perovskite oxide, demonstrating a plastic strain up to ~7% under uniaxial bulk compression. Owing to its prototypical nature in condensed matter physics^{18,19} and its role as a model electronic oxide, SrTiO₃ has been extensively studied thereafter for its dislocation plasticity, ranging from macroscale²⁰ and mesoscale^{21,22} to nanoscale.^{23–26} Later in 2016, Mark et al.²⁷ reported *unexpected* bulk plasticity in single-crystal KNbO₃, which is orthorhombic (pseudo-cubic) at room temperature.²⁸ This finding in KNbO₃ was further confirmed by Höfling et al. in 2021²⁹ and Preuß et al. in 2023.³⁰ So far, SrTiO₃ and KNbO₃ have remained the only two perovskite oxides reported in the literature regarding room-temperature bulk plasticity.

In light of the increasing interest in using dislocations as one-dimensional line defects in ceramic oxides to harvest both functional and mechanical properties,^{31,32} there is a pressing need to seek more room-temperature ductile ceramics as well as to engineer dislocations into such functional oxides for harnessing dislocation-tuned properties. Recently, we achieved this by developing an experimental toolbox for tuning dislocation densities and plastic zone sizes,³³ for example, in SrTiO₃. However, the pursuit of finding more room-temperature ductile ceramics remains largely unexplored so far. With the abundant techniques and experimental protocols recently established for room-temperature dislocation engineering,³³ we begin our quest to discover other ceramics that can be plastically deformed at room temperature at meso-/macroscale.

Here we report the third ductile perovskite oxide (potassium tantalate oxide, KTaO₃), independent of Khayr et al.,³⁴ on its room-temperature plasticity, with tunable dislocation densities and plastic zone size using a mechanics-based combinatorial experimental approach via cyclic Brinell indentation, scratching, and uniaxial bulk compression. KTaO₃ recently received much attention, owing to its potential for functional oxide electronics^{35,36} and tunable ferroelectricity that is achieved through Nb doping.³⁷ These physical properties extend applications of KTaO₃ toward piezocatalysis, pyrocatalysis,³⁸ and photocatalysis.^{39,40} Dislocations represent an additional degree of freedom that translates into all these applications, and it is therefore likely to spark more research interest in dislocation-tuned functional properties in KTaO₃.

2 | EXPERIMENTAL PROCEDURE

For cyclic Brinell indentation and scratching tests, a sample with a geometry of ~1×5×5 mm was used. The synthetic undoped single-crystal KTaO₃ sample was prepared by solidification from a nonstoichiometric melt in Oak Ridge National Laboratory. The tests were run on a universal hardness tester (Finotest; Karl-Frank GmbH), following the experimental procedure established by the current authors.^{21,22} The indenter was mounted with a Brinell indenter with a diameter of 2.5 mm (hardened steel ball; Habu Hauck Prüftechnik GmbH) and a movable stage (Physik Instrumente GmbH & Co. KG). For both cyclic indentation and scratching tests, a dead weight of 1 kg was used. For scratching tests, a speed of 0.5 mm/s (lateral motion) was adopted. Additionally, silicone oil was used as a lubricant to reduce the indenter wear and to suppress sample crack formation. After mechanical deformation, the sample was cleaned with acetone and dried in air. The surface slip traces in the plastic zones were visualized using a laser confocal microscope (LEXT OLS4000;

Olympus IMS). Dark-field imaging mode was used on a Zeiss optical microscope (Zeiss Axio Imager2; Carl Zeiss AG) to exclude potential crack formation underneath the surface.

For uniaxial bulk compression, single-crystal samples (Hefei Single Crystal Material Technology) with a dimension of 3×3×6 mm were used. The long axis of the samples was aligned in the <001> direction. The samples were six-sided polished to mirror finish to minimize surface damage. Uniaxial compression was performed with a constant strain rate of $1.5 \times 10^{-4} \text{ s}^{-1}$ (MTS E45). The deformation images were collected in the VIC-gauge 2D software (Correlated Solution, Inc.). Before compression, two Al₂O₃ plates were placed on top and bottom of the KTaO₃ specimen to offer smoother contact surfaces.

To visualize the dislocation structures in the plastic zone, transmission electron microscopy (TEM) lamellae were lifted out along the scratching direction using a focused ion beam (FIB). The lamellae with a thickness of ~80 nm were prepared and thinned by a FIB (Helios Nanolab 600i, FEI). Microstructures of KTaO₃ including dislocations were characterized by a 200 kV-TEM (FEI Talos F200X G2, Thermo Fisher Scientific, USA) with STEM mode. The annular bright field-scanning transmission electron microscopy (ABF-STEM) images were collected with inner and outer semi-collection angles of 12–20 mrad.

3 | RESULTS AND ANALYSES

3.1 | Brinell indentation and scratching

Figure 1A–C demonstrates the surface plastic deformation after 1 cycle (1x) and 10 cycles (10x) Brinell indentation. The surface slip traces are aligned vertically and horizontally after 1x and 10x indentation (Figure 1A), and the slip trace number increases from 1x to 10x indentation (Figure 1B). The depth profiles of these two indentation imprints in Figure 1C (corresponding to the two yellow dashed lines in Figure 1A,B) indicate a maximum depth of ~120 nm after 1x and ~220 nm after 10x indentation. The plastic zone size in both cases has a diameter of ~150 μm, suggesting that the surface is nominally flat in the indented region.

In addition to the cyclic Brinell indentation test, cyclic scratching tests were performed using the same indenter. Figure 1D,E reveals an increase in the slip trace densities with the increasing scratching number from 1x to 10x. For scratching, each cycle is defined as one traversal. The maximum depth of the scratch tracks (Figure 1F, corresponding to the two yellow dashed lines in Figure 1D,E) was measured to increase from ~100 nm (1x) up to ~250 nm (10x).

Different from the sink-in feature in the 1x scratching as well as the 1x and 10x indentation imprints, the 10x scratching depth profile exhibits two shoulders (pile-up, indicated by the two red arrows in Figure 1F). This pile-up was likely caused by the “plastic plowing” of the material by the spherical indenter during the back-and-forth cyclic scratching (scratching directions indicated by the yellow arrows in Figure 1E). This pile-up is strong evidence of good room-temperature plastic deformation of this material.

To rule out the possible cracking underneath the indentation imprints/scratch track, dark-field imaging mode (sensitive to under-surface cracks, featured as white contrasts) was used. No visible cracks were found up to 25 cycles of scratching. This observation is consistent with the results obtained on other ductile oxides (e.g., SrTiO₃^{21,22}) at room temperature. Worth mentioning is that both the Brinell ball indentation and scratching test results in KTaO₃ closely resemble the slip trace features in SrTiO₃ with the same (001) surface being deformed. The plastic zone size is also almost identical for KTaO₃ observed here as in SrTiO₃²¹ under the same loading conditions. Such similarities suggest that the lattice friction stress in KTaO₃ shall be sufficiently low to allow easy dislocation glide and multiplication at room temperature. Note that single-crystal SrTiO₃ was reported to plastically yield around 110–150 MPa during bulk compression along the [001] orientation (summarized literature results by Stich et al.⁴¹). If the deformation behavior is similar for these two perovskite oxides, then the yield strength of single-crystal KTaO₃ should be around the same range. To this end, further validation with uniaxial bulk compression was performed on KTaO₃ along the [001] direction.

3.2 | Uniaxial bulk compression

The engineering stress-strain curve in Figure 2A and the deformation process in Figure 2B demonstrate the bulk plastic deformation. Unlike the room-temperature bulk stress-strain curves in SrTiO₃^{17,42} and KNbO₃,^{27,29} here for KTaO₃ it exhibits an upper yield point and a lower yield point (indicated in Figure 2A). The upper yield point (Figure 2A) is $\sigma_{y_up} = 274 \text{ MPa}$ and the lower yield point is $\sigma_{y_low} = 250 \text{ MPa}$. This load drop behavior is not uncommon for ceramics that undergo plastic deformation. For instance, similar yield behavior was reported in bulk compression of sapphire at high temperature⁴³ and discussed in single-crystal LiF at room temperature.⁴⁴ Due to the initially low mobile dislocation density in such ceramic crystals, dislocation multiplication was proposed to have caused such a stress drop instead of due to the unpinning of

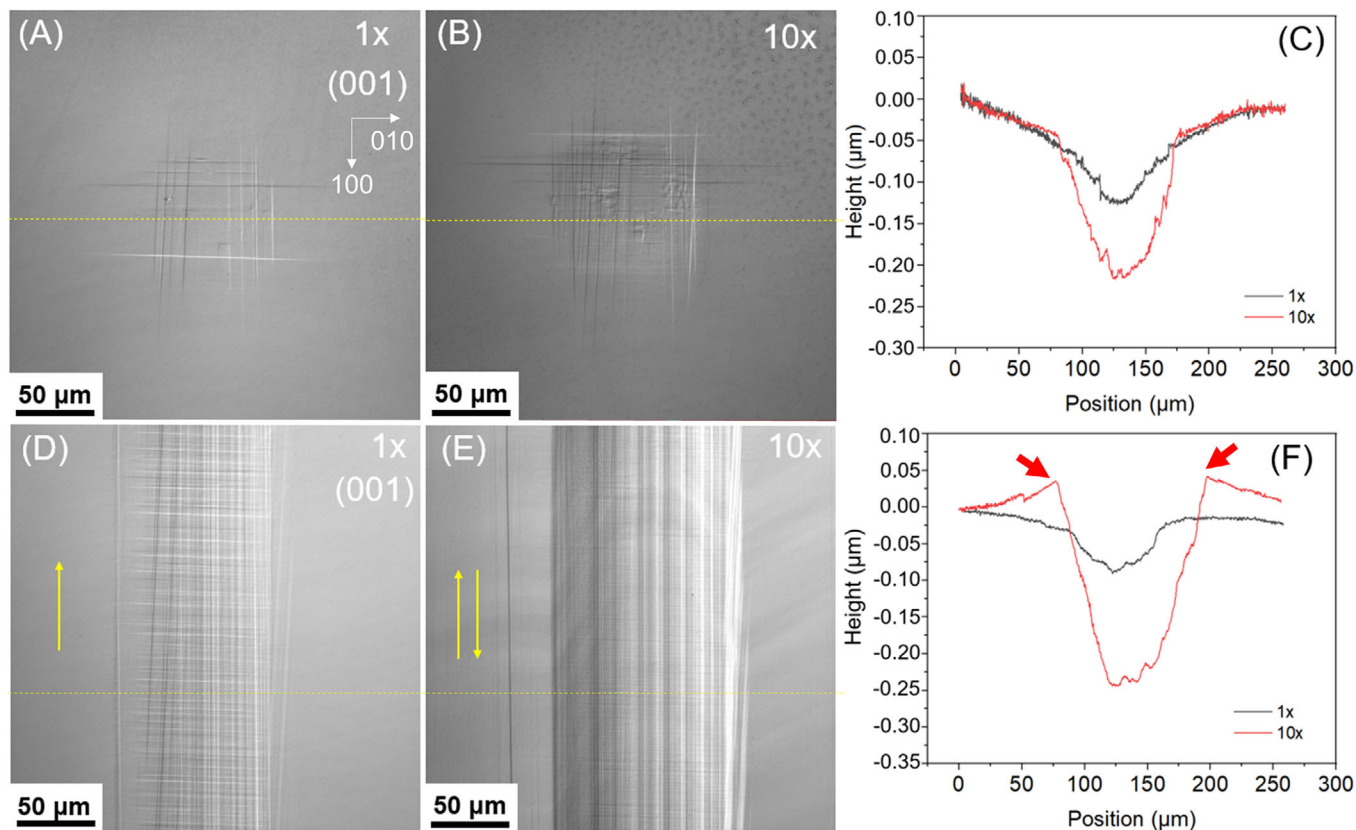


FIGURE 1 Laser microscope images featuring the plastic deformation on the (001) surface after Brinell ball indentation (A, B) and scratching (D, E). Note 1x and 10x stand for 1-cycle and 10-cycle deformation, respectively. The yellow arrows in (D, E) indicate the scratching direction. Depth profiles (C, F) corresponding to the yellow dashed lines were extracted, with the unperturbed sample surface corresponding to the zero point in the y-axis.

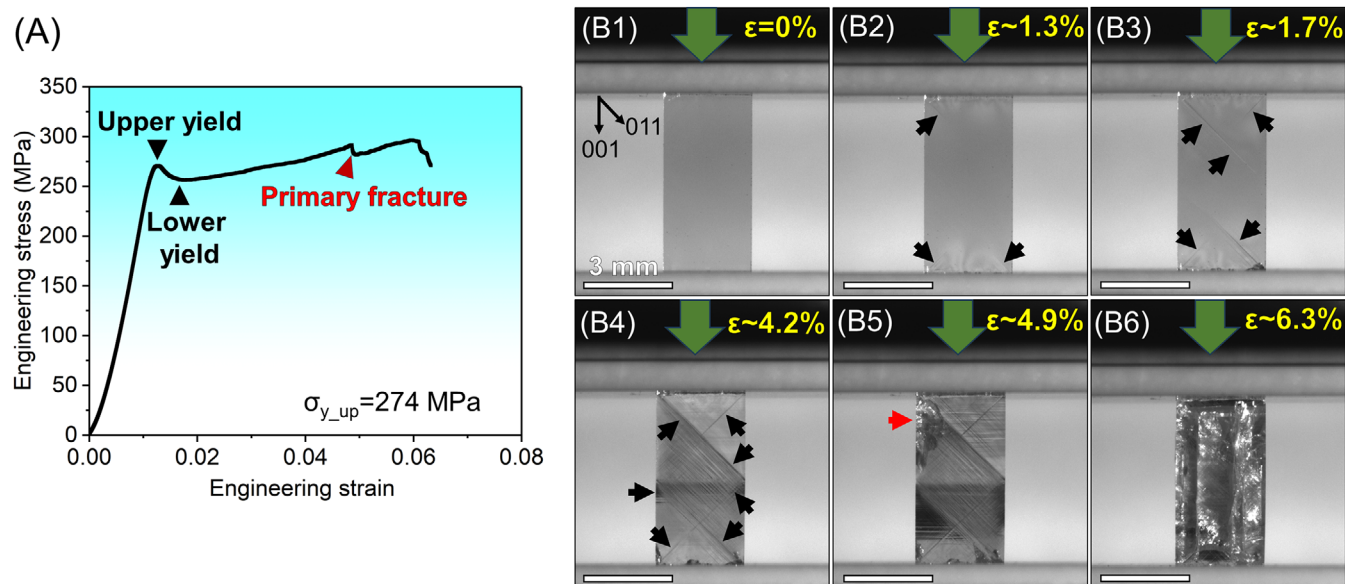


FIGURE 2 Bulk compression of single-crystal KTaO₃ along the <001> direction: (A) engineering stress-strain curve; (B1–B6) Screenshots of the in-situ bulk compression at different strains. The black arrows indicate the slip traces and the red arrow indicates the crack formation. The scale bar in (B1) is consistent for all six sub-figures.

a Cottrell cloud as in the case of α -iron, where dislocation pinning results from the impurities such as carbon.⁴⁵

Following the upper yield point and then the lower yield point, the stress increased from 250 MPa (i.e., the lower yield point in Figure 2A) up to \sim 300 MPa, where another load drop was observed (red arrow in Figure 2A). On the one hand, the stress increase after the lower yield point indicates work hardening behavior, as evidenced by the increased number of slip traces (dark lines that lie 45° to the loading axis), indicated by the black arrows in Figure 2B3–B4. These slip traces confirm that the dislocation glide occurs on the $\{110\}$ planes. On the other hand, the load drop (red arrow in Figure 2A) was found to correspond to the primary fracture event observed by the in-situ deformation (Figure 2B5, where the bright features on the top right corner indicate a main crack formed, see the red arrow). The deformed sample was captured (Figure 2B6, at a strain of \sim 6.3%) right before the sample shattered into pieces at a maximum strain of \sim 6.5%. Note the sample in Figure 2B6 is already full of cracks as reflected by the white contrast.

The observed yield stress during bulk compression agrees with the stress analysis using Hertzian contact for the Brinell ball indentation in Figure 1, as will be rationalized in the following. Consider that the post-mortem plastic zone imprint (Figure 1A) has a diameter of $D = 150 \mu\text{m}$, with the load of $P = 1 \text{ kg}$ (9.8 N), we estimate the mean pressure p_0 underneath the indenter to be \sim 555 MPa using the expression $p_0 = P/(\pi D^2/4)$.⁴⁶ The maximum shear stress (upon plastic yield) during spherical indentation can be calculated according to Swain & Lawn,⁴⁶ giving a value of about $\tau_{max} = 255 \text{ MPa}$ ($0.46p_0$). Note that the critical resolved shear stress (τ_{CRSS}) in the current uniaxial bulk compression is half of the value of the yield strength (here we take the upper yield strength $\sigma_{y,up} = 274 \text{ MPa}$ in Figure 2A), giving $\tau_{CRSS} = 137 \text{ MPa}$. The estimation above is made on the Brinell indentation imprint, which is already in the plastic deformation regime. Consider that Hertzian contact theory is used for elastic deformation, the τ_{max} is expected to be larger than τ_{CRSS} . As both the τ_{max} and τ_{CRSS} are much smaller than the theoretical shear strength (\sim 19 GPa for KTaO_3 , estimated by $G/2\pi$, G is the shear modulus) for homogeneous dislocation nucleation, this suggests that the plastic deformation under the large Brinell indenter as well as the uniaxial bulk compression is mediated by dislocation multiplication and dislocation glide. It is thus expected that the lattice friction stress for dislocation glide in KTaO_3 at room temperature shall be close to $\tau_{CRSS} = 137 \text{ MPa}$ (which is likely an upper bound). This value is higher but close to that in SrTiO_3 (\sim 90 MPa⁴⁷) and KNbO_3 (\sim 30 MPa^{27,29}).

3.3 | TEM characterization of dislocations

To directly prove that the dislocation densities in the plastic zone can be tuned via dislocation multiplication by increasing the number in the deformation cycles, we performed TEM analysis in the 1x and 10x scratched regions. As illustrated in Figure 3A, there are a few dislocations with long segments in the area of view after 1x scratching. These long segments are aligned on the $\{110\}$ planes. This is consistent with the slip trace observation during bulk deformation (Figure 2B). After 10x scratching, the dislocation density increased dramatically and the dislocation lines were heavily tangled up with each other, where the dislocation density is estimated to be higher than $10^{14}/\text{m}^2$. Although the majority of the dislocations are still projected in the $\langle 110 \rangle$ directions, many short and curved dislocation segments are generated. These features are a result of the cyclic scratching, which strongly promotes dislocation multiplication and interaction. Such profuse dislocation multiplication significantly increases the dislocation plasticity, which is in line with the observation of the pile-up behavior after 10x Brinell ball scratching. Further analysis of the Burgers vector and the line vector of the dislocations suggest a Burgers vector of $\langle 110 \rangle$ and both edge and screw types of dislocations are generated. It is thus confirmed that KTaO_3 has the same slip system as in the case of SrTiO_3 ¹⁸ and KNbO_3 (pseudo-cubic),²⁷ namely, the $\langle 110 \rangle \{1\bar{1}0\}$ slip systems are activated at room temperature.

4 | DISCUSSION

Single-crystal KTaO_3 was reported to be very susceptible to brittle cleavage along the (001) surface.⁴⁸ Independent of the current work, Khayr et al.³⁴ studied the dislocation structural properties of plastically deformed KTaO_3 without direct visualization of the deformation features such as slip traces (Figures 1,2) and dislocation mesostructures (Figure 3). Here we present compelling evidence of room-temperature plasticity in single-crystal KTaO_3 , with successful dislocation engineering at both the mesoscale and the bulk scale without inducing visible cracks. This crack suppression is attributed to the profuse dislocation multiplication and good dislocation mobility under the blunt spherical Brinell indenter, which proves to be more advantageous than pyramidal indenters such as Vickers indenter that is widely used for indentation fracture toughness evaluation in brittle solids.^{49,50}

The choice of KTaO_3 was made based on its structural and atomic similarities to the other two ductile

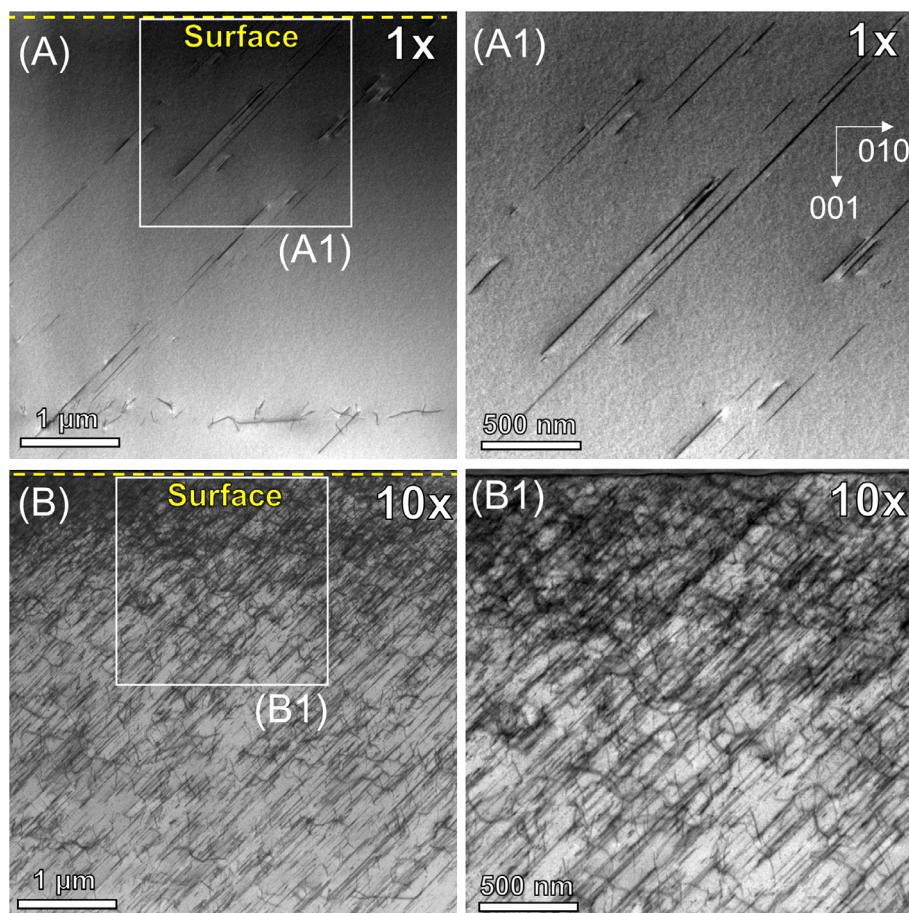


FIGURE 3 Visualization of dislocations (dark lines) in annular bright field-scanning transmission electron microscopy (ABF-STEM): (A) after 1x scratching; (B) after 10x scratching. The dislocation density is tunable depending on the number of cyclic scratching. The orientations in (A1) are consistent for all four sub-figures.

perovskite oxides SrTiO_3 and KNbO_3 . KTaO_3 has a cubic structure at room temperature similar to SrTiO_3 , also Ta and Nb have the same ionic radii of 0.64 Å (for +5 charge state and 6-fold coordination).⁵¹ This led to our original hypothesis that KTaO_3 might also be ductile at room temperature, like SrTiO_3 and KNbO_3 . At this stage, the underlying mechanisms for yielding such dislocation plasticity in KTaO_3 remain unclear. Nevertheless, considering that KTaO_3 , SrTiO_3 , and KNbO_3 are very similar in crystal structure and much often used together for comparison in their physical properties,³⁵ it is likely that the dislocation mechanisms in these materials are similar, particularly concerning the dislocation core structure. For instance, TEM observations and atomistic simulations in SrTiO_3 ^{52,53} as well as in KNbO_3 ²⁸ suggest that the dislocations are dissociated into partials, which facilitates good dislocation mobility at room temperature. To confirm if this is the case for KTaO_3 , future work will involve high-resolution TEM characterization as well as molecular dynamics simulations in this direction.

It is worth noting that, due to the earlier discovery of room-temperature bulk dislocation plasticity and the simple dislocation introduction process in SrTiO_3 , most of the dislocation-based functional and mechanical properties studies^{54–56} have been reported using this model material. Now with the simple and efficient dislocation engineering demonstrated here in KTaO_3 , and considering that KTaO_3 has been deemed as the “new kid on the spintronics block”,³⁵ it is expected that our finding will serve as a fundamental building block for upcoming versatile studies in KTaO_3 tuned by dislocations.

5 | CONCLUSION

We found that single-crystal KTaO_3 with a cubic structure can be plastically deformed at room temperature via bulk uniaxial compression, Brinell ball indentation, and scratching. The room-temperature slip systems in KTaO_3 are identified to be $\langle 110 \rangle \{1\bar{1}0\}$, the same as those observed in SrTiO_3 and KNbO_3 deformed at room temperature.

For the single crystals compressed along the $\langle 001 \rangle$ direction in this work, the bulk yield strength of KTaO_3 was ~ 274 MPa, and the critical resolved shear stress is estimated to be ~ 137 MPa (likely the upper bound) to move the dislocations. Unlike the discrete slip bands generated during bulk compression, the Brinell ball indentation and scratching generate continuous plastic zones extending up to hundreds of micrometers with dislocation densities exceeding $\sim 10^{14}/\text{m}^2$ after 10-cycle scratching. It remains an open question at this stage to pinpoint the fundamental mechanisms responsible for the room-temperature dislocation plasticity in KTaO_3 . Our findings are expected to open new avenues to investigate dislocation-tuned mechanical and functional properties in KTaO_3 .

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REFERENCES

- Basu S, Barsoum MW. Deformation micromechanisms of ZnO single crystals as determined from spherical nanoindentation stress-strain curves. *J Mater Res*. 2007;22(9):2470–77.
- Page TF, Oliver WC, McHargue CJ. The deformation behavior of ceramic crystals subjected to very low load (nano)indentations. *J Mater Res*. 2011;7(2):450–73.
- Fang X, Bishara H, Ding K, Tsybenko H, Porz L, Höfling M, et al. Nanoindentation pop-in in oxides at room temperature: dislocation activation or crack formation? *J Am Ceram Soc*. 2021;104:4728–41.
- Korte-Kerzel S. Microcompression of brittle and anisotropic crystals: recent advances and current challenges in studying plasticity in hard materials. *MRS Commun*. 2017;7(2):109–20.
- Fujikane M, Nagao S, Chrobak D, Yokogawa T, Nowak R. Room-temperature plasticity of a nanosized GaN crystal. *Nano Lett*. 2021;21(15):6425–31.
- Gilman JJ, Johnston WG. Observations of dislocation glide and climb in lithium fluoride crystals. *J Appl Phys*. 1956;27(9):1018–22.
- Johnston WG, Gilman JJ. Dislocation velocities, dislocation densities, and plastic flow in lithium fluoride crystals. *J Appl Phys*. 1959;30(2):129–44.
- Johnston WG, Gilman JJ. Dislocation multiplication in lithium fluoride crystals. *J Appl Phys*. 1960;31(4):632–43.
- Higashida K, Narita N, Matsunaga K. Effect of dislocation activities on crack extension in ionic crystals. *Mater Sci Eng, A*. 1994;176:147–53.
- Higashida K, Narita N, Matsunaga K, Onodera R. Effects of low energy dislocation structures on crack tip shielding in ionic crystals. *Phys Stat Sol A*. 1995;149:429–43.
- Whitworth RW. Charged dislocations in ionic crystals. *Adv Phys*. 1975;24(2):203–304.
- Gorum AE, Parker ER, Pask JA. Effect of surface conditions on room-temperature ductility of ionic crystals. *J Am Ceram Soc*. 1958;41(5):161–64.
- Stokes RJ, Johnston TL, Li CH. Crack formation in magnesium oxide single crystals. *Philos Mag*. 1958;3(31):718–25.
- Cordier P, Amodeo J, Carrez P. Modelling the rheology of MgO under Earth's mantle pressure, temperature and strain rates. *Nature*. 2012;481(7380):177–80.
- Gaillard Y, Tromas C, Woignard J. Quantitative analysis of dislocation pile-ups nucleated during nanoindentation in MgO . *Acta Mater*. 2006;54(5):1409–17.
- Oshima Y, Nakamura A, Matsunaga K. Extraordinary plasticity of an inorganic semiconductor in darkness. *Science*. 2018;360:772–74.
- Brunner D, Taeri-Baghdarani S, Sigle W, Rühle M. Surprising results of a study on the plasticity in strontium titanate. *J Am Ceram Soc*. 2001;84(5):1161–63.
- Gumbsch P, Taeri-Baghdarani S, Brunner D, Sigle W, Rühle M. Plasticity and an inverse brittle-to-ductile transition in strontium titanate. *Phys Rev Lett*. 2001;87(8):085505.
- Gao P, Yang S, Ishikawa R, Li N, Feng B, Kumamoto A, et al. Atomic-scale measurement of flexoelectric polarization at SrTiO_3 dislocations. *Phys Rev Lett*. 2018;120(26):267601.
- Taeri S, Brunner D, Sigle W, Rühle M. Deformation behaviour of strontium titanate between room temperature and 1800 K under ambient pressure. *Int J Mater Res*. 2004;95(6):433–46.
- Okafor C, Ding K, Zhou X, Durst K, Rödel J, Fang X. Mechanical tailoring of dislocation densities in SrTiO_3 at room temperature. *J Am Ceram Soc*. 2022;105:2399–402.
- Fang X, Preuß O, Breckner P, Zhang J, Lu W. Engineering dislocation-rich plastic zones in ceramics via room-temperature scratching. *J Am Ceram Soc*. 2023;106:4540–45.

23. Javaid F, Bruder E, Durst K. Indentation size effect and dislocation structure evolution in (001) oriented SrTiO₃ Berkovich indentations: HR-EBSD and etch-pit analysis. *Acta Mater.* 2017;139:1–10.
24. Javaid F, Stukowski A, Durst K. 3D Dislocation structure evolution in strontium titanate: spherical indentation experiments and MD simulations. *J Am Ceram Soc.* 2017;100(3):1134–45.
25. Fang X, Ding K, Janocha S, Minnert C, Rheinheimer W, Frömling T, et al. Nanoscale to microscale reversal in room-temperature plasticity in SrTiO₃ by tuning defect concentration. *Scr Mater.* 2020;188:228–32.
26. Fang X, Ding K, Minnert C, Nakamura A, Durst K. Dislocation-based crack initiation and propagation in single-crystal SrTiO₃. *J Mater Sci.* 2021;56:5479–92.
27. Mark AF, Castillo-Rodriguez M, Sigle W. Unexpected plasticity of potassium niobate during compression between room temperature and 900°C. *J Eur Ceram Soc.* 2016;36(11):2781–93.
28. Hirel P, Mark AF, Castillo-Rodriguez M, Sigle W, Mrovec M, Elsässer C. Theoretical and experimental study of the core structure and mobility of dislocations and their influence on the ferroelectric polarization in perovskite KNbO₃. *Phys Rev B.* 2015;92(21):214101.
29. Hoefling M, Trapp M, Porz L, Ursic H, Bruder E, Kleebe H-J, et al. Large plastic deformability of bulk ferroelectric KNbO₃ single crystals. *J Eur Ceram Soc.* 2021;41:4098–107.
30. Preuß O, Bruder E, Lu W, Zhuo F, Minnert C, Zhang J, et al. Dislocation toughening in single-crystal KNbO₃. *J Am Ceram Soc.* 2023;106:4371–81.
31. Ikuhara Y. Nanowire design by dislocation technology. *Prog Mater Sci.* 2009;54(6):770–91.
32. Fang X, Nakamura A, Rödel J. Deform to perform: dislocation-tuned properties of ceramics. *Am Ceram Soc Bull.* 2023;102(5):24–29.
33. Fang X. Mechanical tailoring of dislocations in ceramics at room temperature: a perspective. *J Am Ceram Soc.* 2024;107(3):1425–47.
34. Khayr I, Hameed S, Budić J, He X, Spieker R, Najev A, et al. Structural properties of plastically deformed SrTiO₃ and KTaO₃. *arXiv.* 2024. <https://doi.org/10.48550/arXiv.2405.13249>
35. Gupta A, Silotia H, Kumari A, Dumen M, Goyal S, Tomar R, et al. Chakraverty, KTaO₃ – the new kid on the spintronics block. *Adv Mater.* 2022, 34(9):e2106481.
36. Vicente-Arche LM, Brehin J, Varotto S, Cosset-Cheneau M, Mallik S, Salazar R, et al. Spin-charge interconversion in KTaO₃ 2D electron gases. *Adv Mater.* 2021;33(43):e2102102.
37. Toulouse J, Wang XM, Boatner LA. Elastic anomalies at the cubic-tetragonal transition in KTN. *Solid State Commun.* 1988;68:353–56.
38. Wang M, Wang B, Huang F, Lin Z. Enabling PIEZOpotential in PIEZOelectric semiconductors for enhanced catalytic activities. *Angew Chem.* 2019;58(23):7526–36.
39. Grabowska E. Selected perovskite oxides: Characterization, preparation and photocatalytic properties—a review. *Appl Catal B.* 2016;186:97–126.
40. Kakekhani A, Ismail-Beigi S, Altman EI. Ferroelectrics: A pathway to switchable surface chemistry and catalysis. *Surf Sci.* 2016;650:302–16.
41. Stich S, Ding K, Muhammad QK, Porz L, Minnert C, Rheinheimer W, et al. Room-temperature dislocation plasticity in SrTiO₃ tuned by defect chemistry. *J Am Ceram Soc.* 2022;105:1318–29.
42. Brunner D. Low-temperature plasticity and flow-stress behaviour of strontium titanate single crystals. *Acta Mater.* 2006;54(19):4999–5011.
43. Firestone RF, Heuer AH. Yield point of sapphire. *J Am Ceram Soc.* 2006;56(3):136–39.
44. Gilman JJ, Johnston WG. Behavior of individual dislocations in strain-hardened LiF crystals. *J Appl Phys.* 1960;31(4):687–692.
45. Cottrell AH, Bilby BA. Dislocation theory of yielding and strain ageing of iron. *Proc Phys Soc Sect A.* 1949:49–62.
46. Swain MV, Lawn BR. A study of dislocation arrays at spherical indentations in LiF as a function of indentation stress and strain. *Phys Stat Sol.* 1969;35:909–23.
47. Javaid F, Johanns KE, Patterson EA, Durst K. Temperature dependence of indentation size effect, dislocation pile-ups, and lattice friction in (001) strontium titanate. *J Am Ceram Soc.* 2018;101(1):356–64.
48. Setvin M, Reticcioli M, Poelzleitner F, Hulva J, Schmid M, Boatner LA, et al. Polarity compensation mechanisms on the perovskite surface KTaO₃ (001). *Science.* 2018;359:572–75.
49. Anstis GR, Chantikul P, Lawn BR, Marshall DB. A critical evaluation of indentation techniques for measuring fracture toughness: I, direct crack measurements. *J Am Ceram Soc.* 1981;64(9):533–38.
50. Lee JH, Gao YF, Johanns KE, Pharr GM. Cohesive interface simulations of indentation cracking as a fracture toughness measurement method for brittle materials. *Acta Mater.* 2012;60(15):5448–67.
51. Shannon RD. Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides. *Acta Cryst A.* 1976;32:751–67.
52. Matsunaga T, Saka H. Transmission electron microscopy of dislocations in SrTiO₃. *Philos Mag Lett.* 2000;80(9):597–604.
53. Klomp AJ, Porz L, Albe K. The nature and motion of deformation-induced dislocations in SrTiO₃: Insights from atomistic simulations. *Acta Mater.* 2023;242:118404.
54. Kissel M, Porz L, Frömling T, Nakamura A, Rödel J, Alexe M. Enhanced photoconductivity at dislocations in SrTiO₃. *Adv Mater.* 2022;2203032.
55. Hameed S, Pelc D, Anderson ZW, Klein A, Spieker RJ, Yue L, et al. Enhanced superconductivity and ferroelectric quantum criticality in plastically deformed strontium titanate. *Nat Mater.* 2022;21:54–61.
56. Szot K, Speier W, Bihlmayer G, Waser R. Switching the electrical resistance of individual dislocations in single-crystalline SrTiO₃. *Nat Mater.* 2006;5(4):312–20.

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