Atomic scale study of oxygen annealing effect on piezoelectricity enhancement of $(K,Na)NbO_3$ nanorods

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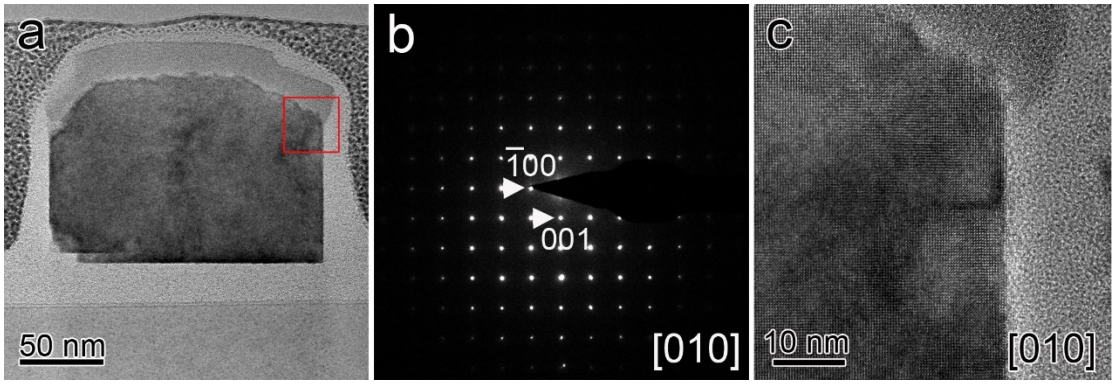

Fig. S1. (a) TEM image of the cross-section of a specific as-grown KNN nanorod showing an approximate rectanglar shape. (b) Corresponding SAED pattern of the cross-section, which indicates the growth direction of [010], and the bounding surfaces of (100) and (001) for the KNN nanorod. (c) HRTEM image of the red box region in (a).

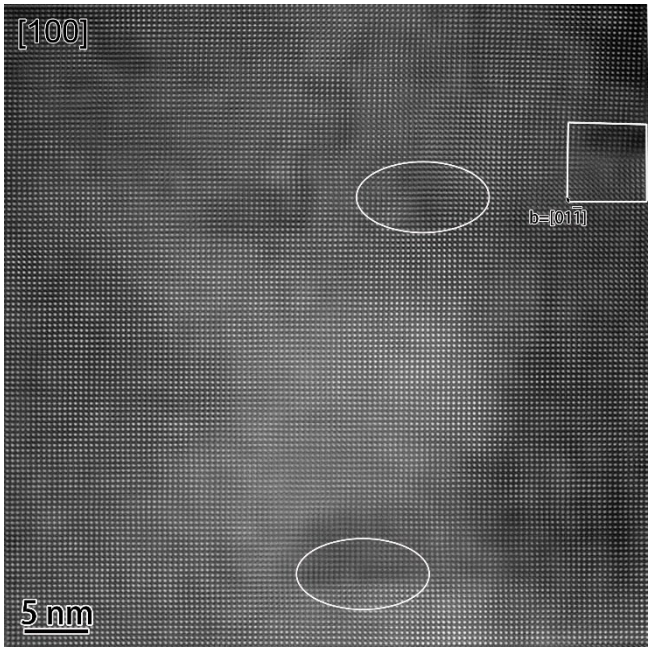

Fig. S2. High-resolution HAADF image of specific as-grown KNN nanorod projected along [100] direction, and the region is far away from the KNN/STO interface. The white ellipses circle out regions including stacking fault. The rectangle is Burgers circuit surrounding an edge dislocation, and the Burgurs vector is determined to be [$01\bar{1}$].

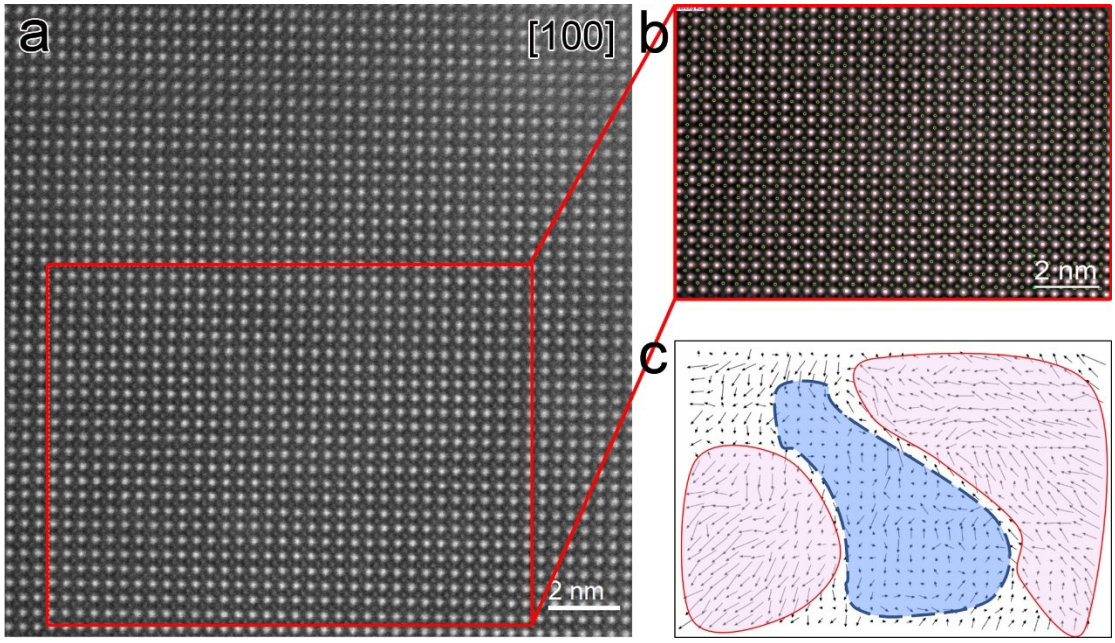

Fig. S3. (a) High-resolution HAADF image recorded from an as-grown KNN nanorod, and the region including a 90° domain is framed in a red box. (b) Image of the red box region in (a) with the exact position of each atomic column determined by peak-finding algorithm. (c) The map of displacement vectors (NbO_2 → K/Na) showing the existence of a 90° domain boundary.

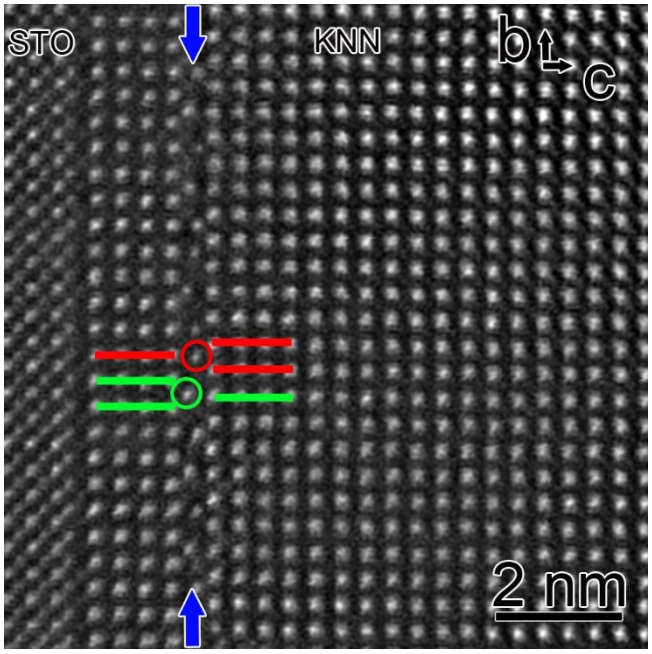

Fig. S4. Atomic-resolution HAADF image recorded from the annealed KNN/STO interface showing an anti-phase boundary in the KNN region, as indicated by blue arrows. The Nb atoms (marked by circles) within the boundary show a zigzag distribution along the vertical direction.

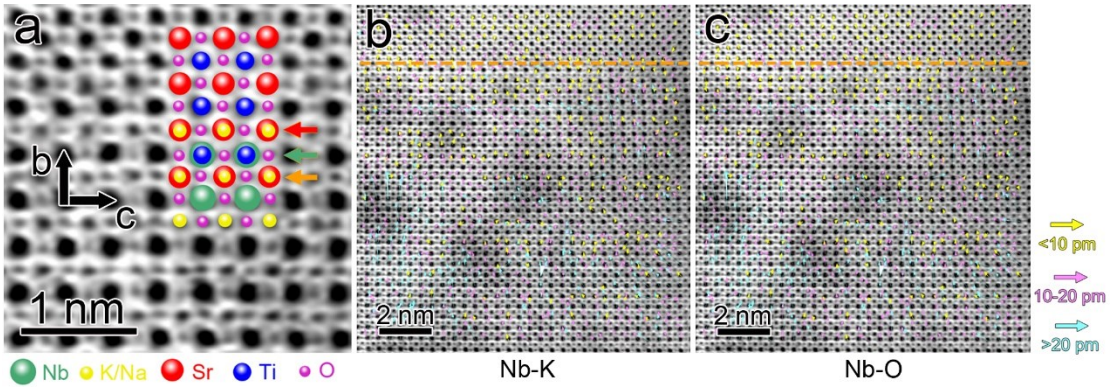

Fig. S5. (a) High-resolution ABF image of the annealed KNN/STO interface, the oxygen atomic columns are clearly observable, and the corresponding atomic model is overlapped for comparison. High-resolution ABF image of a relatively larger area, and the displacement vectors of (b) $NbO_2 \rightarrow$ K/Na and (c) $NbO_2 \rightarrow$ O are overlapped on the ABF image. The different colors indicate different ranges of the length of the vector.

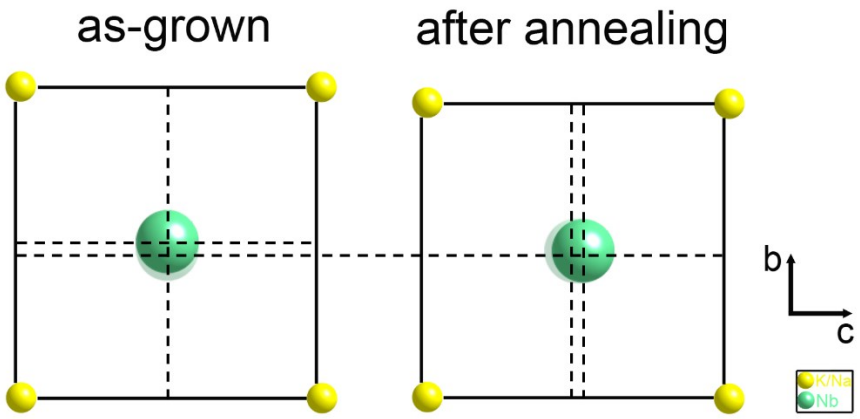

Fig. S6. Schematic of the unit cells of KNN nanorods before and after oxygen annealing using the same axes notation (pseudo-cubic coordination system) based on the measured lattice parameters. The b axis is obviously shrinking, while the c axis is slightly increasing after oxygen annealing. The slight displacements of the Nb atom as compared to the projected equivalent center of the eight nearest K/Na atoms are indicated as well.