High temperature phase transitions in NaNbO$_3$ epitaxial films grown under tensile lattice strain

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We have investigated high temperature phase transitions in NaNbO$_3$ thin films epitaxially grown under tensile lattice strain on (110) DyScO$_3$ substrates using metal-organic vapor phase epitaxy (MOVPE). At room temperature, a very regular stripe domain pattern consisting of the monoclinic $a_1a_2$ ferroelectric phase was observed. Temperature-dependent studies of the refractive index and the optical band gap as well as in situ high-resolution X-ray diffraction (HR-XRD) measurements prove a ferroelectric-ferroelectric phase transition in the range between 250°C and 300°C. The experimental results strongly suggest that the high-temperature phase exhibits a distorted orthorhombic $a_1a_2$ crystal symmetry, with the electric polarization vector lying exclusively in the plane. A second phase transition was observed at about 500°C, which presumably signifies the transition to the paraelectric phase. Both phase transitions show a pronounced temperature-dependent hysteresis, indicating first-order phase transitions.

NaNbO$_3$ based materials have attracted significant interest due to their promising ferro- and piezoelectric properties$^1$ and are thus considered as possible candidates to replace hazardous lead-based materials in piezo-/ferroelectric technological devices. Temperature dependent phase transitions of bulk NaNbO$_3$ have been frequently studied$^{2,3}$ and a complex sequence has been observed in the temperature range from 640°C down to -100°C$^{3,5}$. Above 640°C, NaNbO$_3$ is paraelectric and cubic, while a tetragonal, four orthorhombic, and finally a rhombohedral phase emerges at 640°C, 575°C, 520°C, 480°C, and 100°C during field-free cooling.
respectively. This complexity is a consequence of the coupling of Nb shifts and the octahedral tilting of oxygen around Na. At room temperature NaNbO is antiferroelectric with orthorhombic Pbcm symmetry, however, by applying a weak external electric field or stress it can easily be transformed into a ferroelectric state.

In contrast to bulk NaNbO, hardly any comparable studies can be found for thin films. Thermal phase transitions have been observed for polycrystalline NaNbO films, while for epitaxial films the impact of lattice strains on thermal phase transitions has not yet been studied neither experimentally nor theoretically. On the other hand, for perovskite oxides, strain engineering is an effective tool to tune material properties or even generate properties due the strong coupling between lattice distortions and electronic properties. Lattice strain can be easily imparted to thin films by epitaxial growth and have previously been used to intentionally modify electrical and optical properties as well as to shift the phase transition temperature by hundreds of Kelvin in ferroelectric materials.

The investigation of strain effects requires the epitaxial growth of fully strained films with smooth surface and low defect density. However, deposition of high-quality, stoichiometric epitaxial films of NaNbO is challenging due to the high volatility of the alkali component. Only a few papers have reported the deposition of NaNbO thin films by e.g. pulsed laser deposition and magnetron sputtering. On the other hand, metal-organic vapor phase epitaxy (MOVPE) is a promising deposition technique of high technological relevance. In comparison to physical vapor depositions epitaxial growth takes place close to thermodynamic equilibrium and at comparatively high oxygen partial pressures of typically 10-20 mbar. This provides nearly perfect thin films with smooth surfaces/interfaces and periodic ferroelectric domain patterns.

Recently, we have reported epitaxial growth of high quality NaNbO thin films by MOVPE and found a sequence of phase transitions when the films are grown on various substrates with varying lattice mismatch. In particular, fully compressively strained NaNbO thin films grown on NdGaO substrate exhibit an orthorhombic c phase with exclusive vertical electrical polarization which transforms into the inclined monoclinic Ma phase when the epitaxial strain is partially relaxed. On the other hand, the introduction of tensile strain through epitaxial growth on rare-earth scandates (ReScO) leads to the formation of the monoclinic aia2-phase with pure in-plane electrical polarization. In this study, tensile strained epitaxial NaNbO films have been grown on (110) DyScO (DSO) substrate. In situ high-resolution X-ray diffraction (HRXRD) and spectroscopic ellipsometry (SE) reveal a first-
order phase transition at high temperatures between 250 °C and 300 °C, with a pronounced hysteresis observed between the heating and cooling processes. Although more detailed investigations are still needed, our data at this stage indicate that the high-temperature phase exhibits a distorted $a_1/a_2$ orthorhombic symmetry with pure in-plane polarization.

$\text{NaNbO}_3$ films with a nominal thickness of about 40 nm were grown on 0.1° off-oriented (110) $\text{DyScO}_3$ substrates (CrysTec GmbH Berlin, Source material purity 4 N) by liquid delivery spin MOVPE. Details of the deposition method are given in Ref.18, however, in the present study we use slightly different parameters (Flash evaporation temperature of 230 °C for the Na(thd) (99.999 %) solution and 190 °C for the Nb(EtO)$_5$ (99.999 %) solution, a Na-to-Nb concentration ratio in the source liquids of 4 and an O$_2$-to-Ar ratio of 0.6). Fig. 1a shows an atomic force micrograph (AFM; Bruker Dimension Icon) of such a 40 nm $\text{NaNbO}_3$ film. The surface morphology mimics the step structure of the substrate prior to growth due to 0.1° off-orientation, i.e., it is formed of regularly spaced surface steps, indicating a step-flow growth mode with a very low root mean square (rms) surface roughness of about 0.14 nm. A piezoresponse force microscope (PFM) equipped with a dual AC resonance tracking (DART) mode (Asylum Research MFP-3D stand-alone instrument) was applied to image the ferroelectric domains. Lateral PFM measurements presented in Fig. 1b reveal a periodic stripe domain pattern where the stripes are aligned along the $[1\overline{1}0]_{\text{DSO}}$ direction of the substrate. The bright/yellow and dark/black means that the in-plane polarization vector has a component along the $[1\overline{1}0]_{\text{DSO}}$ and $[1\overline{1}0]_{\text{DSO}}$ directions, respectively. In contrast, the corresponding vertical PFM image (not shown here) exhibits no significant signal, proving that the electric polarization vector is aligned exclusively in the film plane. These results are consistent with the formation of ferroelectric $a_1/a_2$ domains as described in our previous publications14,17,20.

At room temperature the (110) $\text{DyScO}_3$ substrate exhibits an orthorhombic symmetry ($a = 5.4424$ Å, $b = 5.7194$ Å, $c = 7.9043$ Å), with a nearly quadratic surface unit cell with in-plane lattice parameters of 3.948 Å and 3.952 Å along the $[1\overline{1}0]_{\text{DSO}}$ and $[001]_{\text{DSO}}$ directions, respectively. In $\text{Pbcm}$ symmetry, the orthorhombic lattice parameters of NaNbO$_3$ are given by $a_{\text{NNO}} = 5.5047$ Å, $b_{\text{NNO}} = 5.5687$ Å and $c_{\text{NNO}} = 15.523$ Å. For reasons of simplicity, we use the pseudocubic (pc) notation24 with lattice parameters $a_{\text{pc}} = 3.881$ Å and $b_{\text{pc}} = c_{\text{pc}} = 3.915$ Å and $\alpha_{\text{pc}} = 89.34°$ being the angle between the $b_{\text{pc}}$ and $c_{\text{pc}}$ directions (Fig. 1c). The main pseudocubic axes of the epitaxial NaNbO$_3$ film are parallel to the in-plane substrate directions $[1\overline{1}0]_{\text{DSO}}$ and $[001]_{\text{DSO}}$. For more details see Ref.17.
The requirement of elastic energy minimization suggests (100)\textsubscript{pc} orientation of the pseudocubic unit cell of NaNbO\textsubscript{3}. Hence, the NaNbO\textsubscript{3} film experiences anisotropic tensile lattice strain of 0.81\% and 0.94\% in [1\overline{1}0]\textsubscript{DSO} and [001]\textsubscript{DSO} directions, respectively. We have carried out HR-XRD on a Rigaku 9kW SmartLab diffractometer using Cu K\alpha radiation. In Fig. 2a a \(\theta\)–\(\omega\) scan around the symmetrical out-of-plane (110)\textsubscript{DSO} Bragg reflection is shown. The NaNbO\textsubscript{3} film peak appears at slightly larger \(2\theta\) values than the expected bulk values for (100)\textsubscript{pc} and (001)\textsubscript{pc} oriented NaNbO\textsubscript{3} (marked as blue dashed lines) which proves the presence of tensile in-plane strain. Pronounced thickness fringes are observed, attesting that the film surface and film-substrate interface are smooth. A careful analysis leads to a film thickness of \(t = 42.5 \pm 0.5\) nm. Supplementary grazing-incidence in-plane X-ray diffraction in the vicinity of the [1\overline{2}0]\textsubscript{DSO} Bragg reflection (Fig. 2b) shows a clear splitting of the film peaks (P1, P2) as it is characteristic for a (100)\textsubscript{pc} orientation and a monoclinic in-plane shearing of the pseudocubic unit cells axes which is referred to as a\textsubscript{12}\textsubscript{a2} phase\textsuperscript{14,17-20}. From the angular splitting, we were able to determine the in-plane monoclinic angle to be \(\alpha = 89.50^\circ \pm 0.1^\circ\) which fits to the results obtained in Ref.\textsuperscript{14} (see Fig. 4 therein). From the peak width, a mean domain width along [001]\textsubscript{DSO} of about \(w = 18(1)\) nm can be evaluated in agreement with the PFM measurements in Fig. 1b.

The optical properties of the NaNbO\textsubscript{3} thin film were determined by SE using a Woollam M-2000DI rotating compensator ellipsometer in the spectral range of 0.73–6 eV at various angles of incidence 60°, 65° and 70°. To identify the phase transition in the epitaxial NaNbO\textsubscript{3} film, temperature dependent SE measurements were performed from room temperature up to 560 °C. To evaluate the refractive index and band gap energy, we used a model to fit the SE parameters, \(\psi\) and \(\Delta\), which consists of a four-component stack composed of substrate/film/surface roughness/air. The optical properties of the surface roughness layer are analyzed by a Bruggeman effective medium approximation\textsuperscript{25} consisting of a 50\% bulk film/50\% void mixture. An analytical model using Tauc–Lorentz dispersion relations\textsuperscript{26} model was employed to determine the dielectric function and layer thicknesses (see the supplementary material). The TL parameterization is more realistic for the optical functions of amorphous materials\textsuperscript{26}. However, it has been successfully applied to crystalline material\textsuperscript{27,28}. To meet our main objective of detecting the phase transition from temperature dependent SE measurements, we found that the use of TL dispersion is adequate to fit the ellipsometric data of NaNbO\textsubscript{3} film. The obtained film thickness of \(t = (43.5 \pm 0.4)\) nm is in good agreement with the X-ray data (\(t = 42.5 \pm 0.5\) nm) and a surface roughness of about \((0.40 \pm 0.04)\) nm could be determined. Room temperature SE measurements performed at several angles of incidence of 60°, 65° and 70° and
sample orientations (supplementary material, Fig. S1), revealed only a weak dependence of the refractive index (n) and the extinction coefficient (k) (supplementary material Fig. S2), further details are provided in supplementary. Therefore, in the following we focus on results obtained at an angle of incidence of 70°, and an isotropic model was throughout used for all temperature-dependent SE measurements.

Figures 3a and b show the temperature dependence of the real ($\varepsilon_r$) and imaginary ($\varepsilon_i$) parts of the dielectric function, respectively, of the NaNbO$_3$ film as a function of the photon energy. For NaNbO$_3$ the valence band is primarily constituted by the O 2p states, while the conduction band derives from the transition-metal (Nb) d orbitals. The d band consists of a lower energy, wide $d\varepsilon$ sub-band and a higher energy, narrower $d\gamma$ sub-band. The dielectric maximum (imaginary part at 27 °C) at about 5.5 eV is dominated by the valance band $\rightarrow d\varepsilon$ transition$^{29}$. To clarify the shift of the absorption edge around the phase transitions, the imaginary part $\varepsilon_i$ at the absorption edge has been recorded as function of the temperature, as marked (inset of Fig. 3b). The experimental spectra agree with those typically observed in the transparency range of perovskite oxide ferroelectrics and comparable to that of the NaNbO$_3$ film deposited on DyScO$_3$$^{19,29}$. In the near-infrared range, the real part slightly increases with temperature, while at the UV-visible region the imaginary part shows a redshift tendency. This behavior is attributed to electron-phonon interaction that is enhanced with increasing temperature, as observed in other ferroelectric materials$^{30}$.

The evaluated n at 3.2 eV and the band gap energy ($E_g$) of NaNbO$_3$ as a function of temperature on heating and cooling are presented in Figs. 4a and 4b, respectively. The refractive index is graphed at an energy of 3.2 eV, i.e. near the band gap 3.9 eV, to best observe variations with phase transitions and structural changes$^{9,31}$. The refractive index at 3.2 eV of a bare DyScO$_3$ substrate is additionally shown in Fig. 4a as a reference. It reveals a linear dependency as expected for a dielectric material without phase transition. In contrast, the spectra of NaNbO$_3$ show significant deviations from linearity near 305 °C and 520 °C on heating, indicating the occurrence of phase transitions. Furthermore, during the cooling cycle (blue dotted curves), the deviations from linear behavior occur at lower temperatures, resulting in a pronounced hysteresis loop with a width of about 50 K around the phase transitions at 305 °C and 520 °C (Fig. 4).

The band gap energy of NaNbO$_3$ film was estimated from the onset of the main electronic absorption (TL) as well as from the Tauc-plot along the [001]$_{DSO}$ and [110]$_{DSO}$ directions (see the supplementary material for further discussion). Density functional theory calculations of the
electronic properties of orthorhombic NaNbO$_3$ revealed that NaNbO$_3$ has an indirect band gap$^{12}$. Therefore, we will discuss the estimated indirect band gap of NaNbO$_3$ film with the reported indirect band gaps. From Table 2 of the supplementary material it is clear that the average of the estimated indirect band gap (Tauc-plot) along the [001] and [1\overline{1}0] directions is (4.04 ± 0.02) eV. This value is larger than the indirect band gap 3.45$^{32}$ eV (Tauc-plot) and 3.39 eV and 3.86$^{33}$ eV estimated using the double TL-dispersion of NaNbO$_3$. Eng et al.$^{34}$ reported that the increase of the Nb–O–Nb bond angle by applying tensile strain leads to an increase of the conduction band width and hence the band gap decreases. However, this has not been observed for our NaNbO$_3$ thin films, where the band gap increases under tensile strain. This increase is tentatively explained by the ferroelectric polarization induced by the tensile lattice strain, which leads to an additional band gap widening$^{35,36}$. On the other hand, the decrease of the band gap with increasing temperature is related to the temperature-dependent dilatation of the lattice whereas the majority contribution comes from the electron lattice interaction$^{37}$. With increasing temperature between room temperature and about 320 °C, and further from 320 °C to 500 °C the decrease of the optical band gap can be fitted by a linear approximation with $\delta E_g/\delta T = -1$ meV/K and $\delta E_g/\delta T = -0.6$ meV/K, respectively, these values are in good agreement with values of other ferroelectric perovskites$^{38}$. The slight difference between these values additionally indicates the existence of two different phases in this temperature range.

To elucidate the structural changes associated with the observed phase transitions, in situ X-ray reciprocal space mappings (RSMs) were recorded from room temperature up to 550 °C. We have chosen the asymmetric (444)$_{DSS}$ substrate Bragg reflection which is sensitive to both vertical and horizontal normal strain components as well as to shear strains. In this scattering geometry the in-plane component $Q_x$ of the scattering vector is parallel to the [001]$_{DSS}$ direction of the DyScO$_3$ substrate while the out-of-plane component $Q_z$ is oriented along the surface normal of the (110)$_{DSS}$ plane. Selected RSMs presented in Fig. 5a-f reveal the following sequence:

(i) From room temperature up to 300 °C, a single film Bragg reflection is observed which occurs at larger vertical scattering component $Q_z$ but identical horizontal scattering component $Q_x$ as the (444)$_{DSS}$ substrate Bragg reflection. Together with the results from Fig. 1 this is in accordance with the presence of an a$_{1}a_{2}$ phase in the films and proves that the film is fully tensile strained on the DyScO$_3$ substrate.

(ii) Increasing the temperature to 320 °C the film peak exhibits a pronounced horizontal splitting. This is attributed to a change of the thin film crystal symmetry and indicates a structural phase transition between 300 °C and 320 °C, which is in good agreement with...
the SE measurements (Fig. 4). The center of mass of the doubled film peaks is slightly shifted towards larger \( Q_x \) values as compared to the substrate peak, indicating a slightly reduced horizontal lattice spacing.

(iii) The horizontal splitting persists up to 500 °C, while above 500 °C it disappears, leaving a single film peak that appears at identical \( Q_x \) value as the substrate peak. This is a fingerprint of a second structural phase transition at about 500 °C, which fits well to the SE measurements described above in Fig. 4.

(iv) During the cooling cycle (Fig. 5 g-k), the phase transition occurs at lower temperatures. This hysteretic behavior implies a first order phase transition and corresponds well to the behavior of \( n(T) \) and \( E_g(T) \) in Fig. 4.

The horizontal peak splitting displayed in Fig. 5 (e), (g)-(j) indicates the presence of a distorted orthorhombic in-plane \( a_1/a_2 \) ferroelectric phase, similar to the one observed in strained \( K_{0.9}Na_{0.1}NbO_3 \) thin films grown on (110) \( NdScO_3 \) substrate\(^{39,40} \). Indeed, neglecting the octahedral tilting in NaNbO\(_3\) (as opposed to \( K_xNa_{1-x}NbO_3 \) with \( x \geq 0.5 \)), one would expect a similar phase transition path for NaNbO\(_3\) thin film grown on \( DyScO_3 \). A further indication of an exclusively in-plane ferroelectric-to-ferroelectric phase transition (\( a_1a_2 \rightarrow a_1/a_2 \)) can be seen in the behavior of the out-of-plane lattice parameter, which shows no detectable signature across the phase transition. In contrast, such a signature can be detected, for example, in compressively strained \( K_{0.7}Na_{0.3}NbO_3 \) thin films on \( TbScO_3 \), which exhibit a strong vertical polarization component both at room temperature (M\(_c\)-phase) and at high temperatures (c-phase)\(^{13} \). The second phase transition observed at about 500 °C is presumably a transition to the paraelectric phase, which again show a pronounced hysteretic behavior. In any case, further detailed investigations are required for a more accurate characterization of the high-temperature phases.

To conclude, we have investigated tensile strained NaNbO\(_3\) thin films grown by MOVPE on (110) \( DyScO_3 \) substrate. At room temperature we observe a very regular stripe domain pattern consisting of the monoclinic \( a_1a_2 \) ferroelectric phase with exclusive in-plane electrical polarization. Temperature-dependent refractive index and optical band gap measurements as well as \textit{in situ} HR-XRD measurements show a ferroelectric-to-ferroelectric phase transition between 250 °C and 300 °C. Our experimental data strongly suggest that the high temperature phase exhibits a distorted orthorhombic \( a_1/a_2 \) symmetry with pure in-plane polarization presumably along \([1\bar{1}0]_{DyO} \) and \([001]_{DyO} \). In addition, a subsequent phase transition presumably to the paraelectric phase was observed at about 500 °C. For both transitions, a pronounced hysteretic behavior was observed, suggesting first-order phase transitions. Our observations on
strained films differ significantly from the behavior of NaNbO$_3$ bulk crystals, where a much more complicated scenario takes place$^{2,3,5,6}$. Unfortunately, due to the high complexity of the NaNbO$_3$ crystal structure, no corresponding theoretical studies are available so far. For room temperature, only first-principles studies of possible stable ferroelectric phases as a function of strain are available$^{41}$. Recently, these studies have been extended to include anisotropic strain and the tilt of oxygen octahedra$^{42}$. However, there are no calculations of temperature-strain phase diagrams or 3D phase field simulations, which have already been carried out very successfully for the simpler K$_x$Na$_{1-x}$NbO$_3$ ($x \geq 0.5$) material system$^{40,43}$. Our experimental data tentatively show a similar behavior for strained NaNbO$_3$ and K$_x$Na$_{1-x}$NbO$_3$, suggesting that in epitaxial thin films lattice strain has a larger impact on domain formation than octahedral tiltings. A comparison of our experimental data with such 3D phase field simulations would be highly interesting in view of the apparent similarities of the observed phases and phase transitions in strained NaNbO$_3$ and K$_x$Na$_{1-x}$NbO$_3$ thin films.

See the supplementary material for the SE measurements at various angles of incidence, sample rotations and using the interface layer on the model.

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**AUTHOR DECLARATIONS**

Conflict of Interest
The authors have no conflicts of interest to disclose.

DATA AVAILABILITY
The data that support the findings of this study are available from the corresponding authors upon reasonable request.

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Figure captions

FIG. 1. (a) Atomic force micrograph and (b) lateral piezoresponse force micrograph (phase image) of the NaNbO$_3$ strained film grown on (110) DyScO$_3$ substrate (c) Schematic presentation of the orthorhombic (black lines) and inscribed pseudocubic unit cell (blue lines) of NaNbO$_3$ for Pbcm symmetry.

FIG. 2. (a) 2θ-ω scan around the symmetrical (110)$_\text{DyScO}_3$ out-of-plane Bragg reflection. (b) Grazing incidence X-ray diffraction (angular $\phi$-scan) in the vicinity of the (220)$_\text{DyScO}_3$ in-plane Bragg reflection.

FIG. 3. (a) Real ($\varepsilon_r$) and (b) imaginary ($\varepsilon_i$) parts of the dielectric function as a function of photon energy in the epitaxial NaNbO$_3$ film on DyScO$_3$ substrate on heating from 27 °C up to 560 °C.

FIG. 4. (a) Refractive index of NaNbO$_3$ as a function of temperature on heating and cooling and of DyScO$_3$ substrate on heating, (b) optical band gap of NaNbO$_3$ as a function of temperature on heating and cooling.

FIG. 5. X-ray reciprocal space maps of the NaNbO$_3$ film in the vicinity of the asymmetrical (444)$_\text{DyScO}_3$ Bragg reflection of the DyScO$_3$ substrate (a-f) on heating, and, (g-k) on cooling.
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[Diagrams showing X-ray diffraction patterns at various temperatures from 225 °C to 525 °C, with labels indicating 'Heating' and 'Cooling'.]