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# Crystal Structure of $Sr_{0.4}Ce_{0.4}TiO_3$ Ceramics

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A cerium-doped $SrTiO_3$ compound with the composition $Sr_{0.4}Ce_{0.4}TiO_3$ has been produced by conventional solid-state processing. The structure of this compound was analyzed by X-ray, electron, and neutron diffraction. While no superlattice can be observed via X-ray diffraction, both electron and neutron diffraction show evidence of a noncubic supercell caused by antiphase tilting of oxygen octahedra. The most likely space group is $C2/c$, corresponding to an $a^-b^-b^-$ tilt system. Octahedra are tilted by ~5° about the pseudo-cubic $a$-axis and ~1.5° about the pseudo-cubic $b$- and $c$-axes.

## Introduction

It has previously been experimentally verified[1] that charge compensation in cerium-doped $SrTiO_3$ compositions occurs via A-site vacancy formation, with $Ce^{3+}$ dopant cations occupying $Sr^{2+}$ sites and creating A-site vacancies via the reaction

$$Ce_2O_3 \xrightarrow{SrTiO_3} 2Ce^{\bullet\bullet}_{Sr} + V''_{Sr} + 3O^{\times}_{O}$$

These materials typically have dielectric constants in the 113−185 range and quality factors in the range of 6000−11000. As such, they are promising, relatively inexpensive, lead-free candidates for high-permittivity applications (e.g., cellular handsets) in the wireless telecommunications field.

Bamberger et al.[2] first reported the existence of the compound $Sr_2Ce_2Ti_5O_{16}$ and a series of solid solutions of the type $Sr_{2+n}Ce_2Ti_{5+n}O_{16+3n}$ ($n \leq 7$) in 1994; however, the crystal structure and phase purity of these compounds were not well-established. Sreemoolanadhan et al.[3] subsequently reported the microwave dielectric properties of ceramics in this system. Subodh et al.[1] established via X-ray photoelectron spectroscopy (XPS) that the oxidation state of the Ce in such ceramics is chiefly $Ce^{3+}$ rather than $Ce^{4+}$, so the formula is more correctly written as $Sr_{2+n}Ce_2Ti_{5+n}O_{15+3n}$ or, more simply, $Sr_{1-3x/2}Ce_xTiO_3$, where $x = 2/(n + 5)$.

The structure of $Sr_{1-3x/2}Ce_xTiO_3$ ($0.1333 \leq x \leq 0.4$) was initially reported as cubic, $Pm\overline{3}m$, based on X-ray diffraction (XRD) data[1] and vibrational spectroscopy work.[4] Howard et al.[5] investigated the similar $Sr_{1-3x/2}La_xTiO_3$ system and reported a structure in $I4/mcm$ with antiphase octahedral tilting about one axis for $0.2 \leq x < 0.55$. Cation ordering reportedly caused a further transition to $Cmmm$ for $x \geq 0.55$. When the same group[6] later investigated $Sr_{0.1}La_{0.6}TiO_3$, they reported two polymorphs: one ordered in $Cmmm$ and another disordered in $I4/mcm$. Recently, Ubic et al.[7] used a combination of electron and neutron diffraction to investigate the structure of compounds in the $Sr_{1-3x/2}Ce_xTiO_3$ system. At that time, it was found that compositions corresponding to $x = 0.1333$, 0.1667, and 0.25 formed doubled perovskite compounds, with antiphase tilting of oxygen octahedra, in space group $R\overline{3}c$. Similar structures were previously reported for $NdAlO_3$,[8] $LaNiO_3$,[9] $LaAlO_3$,[10,11] $LaCoO_3$,[12−14] and $LaCuO_3$;[15,16] $R\overline{3}c$ was recently reported

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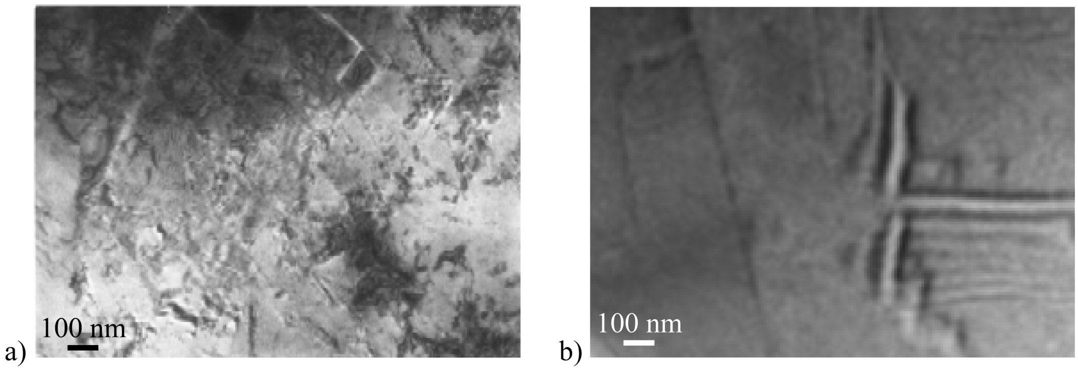

**Figure 1.** (a) Defective grain of $Sr_{0.4}Ce_{0.4}TiO_3$ sintered at 1300 °C for 2 h; (b) less-defective grain of $Sr_{0.4}Ce_{0.4}TiO_3$ sintered at 1400 °C for 2 h.

as the space group of paraelectric $[(Sr_{1-x}Pb_x)_{0.75}Ce_{0.1667}]$-$TiO_3$ ($x < 1/3$).[17] According to both the conventional formula[18] and the revised one recently published by Ubic et al.,[19] the perovskite tolerance factors are high in these materials ($0.9899 \le t \le 1.0716$); however, it has already been established[20] that the tilt system $a^-a^-a^-$ is stabilized by highly charged A-site cations and small tilt angles, both of which conditions characterize all these structures.

Although a fit in $R\bar{3}c$ was also reported[7] for the $x = 0.4$ composition, it was recognized at the time that the fit was poor and a lower-symmetry model would be necessary to fully describe that structure. The current paper presents the results of further refinements of $Sr_{0.4}Ce_{0.4}TiO_3$ and describes that lower-symmetry structure.

## Experimental Methods

$Sr_{1-3x/2}Ce_xTiO_3$ ($x = 0.4$) ceramics were prepared by a conventional solid-state ceramic route. High-purity $SrCO_3$ and $TiO_2$ (99.9+%, Aldrich Chemical Co., Inc., Milwaukee, WI) and $CeO_2$ (99.99%, Indian Rare Earth Ltd., Udyogamandal, India) were used as the starting materials. Stoichiometric amounts of powder mixtures were ball-milled in distilled water medium using yttria-stabilized zirconia balls in a plastic container for 24 h. The slurry was dried, ground, and calcined at 1100 °C for 5 h. The calcined material was then ground into a fine powder and a solution of 4 wt % of poly(vinyl alcohol) (PVA) (molecular weight = 22000, 88% hydrolyzed, BDH Lab Supplies, England) was added dropwise to the dried powders, which were then again ground into fine powder. Cylindrical pellets with a height of ~1−2 mm and a diameter of ~14 mm were made by applying a pressure of 100 MPa. These compacts were then heated to 600 °C for 30 min to burn the binder out before sintering. Pellets of $Sr_{0.4}Ce_{0.4}TiO_3$ were sintered at either 1300 °C for 2 h or 1400 °C for 2 h. Crystal structure and phase purity of the powdered samples were studied by XRD, using nickel-filtered Cu Kα radiation (Rigaku Model D-max X-ray diffractometer, Tokyo, Japan).

Samples for transmission electron microscopy (TEM) were prepared by thinning pellets to electron transparency using conventional ceramographic techniques followed by ion thinning (Model 600, Gatan, Pleasanton, CA) to electron transparency for observation in the TEM system (JEM-2100 HR, JEOL, Tokyo, Japan).

Time-of-flight (ToF) neutron diffraction data were collected for the $Sr_{0.4}Ce_{0.4}TiO_3$ sample on the Neutron Powder Diffractometer (NPDF) at the Manuel Lujan Neutron Scattering Center at Los Alamos National Laboratory. This instrument is a high-resolution powder diffractometer located at flight path 1, 32 m from the spallation neutron target. Powder samples were contained in a vanadium can 0.95 cm in diameter. Absorption was not a problem. The data were collected at room temperature (300 K) using the 148°, 119°, 90°, and 46° banks, which cover a $d$-spacing range of 0.12−7.2 Å. Unit-cell parameters, atomic positions, and isotropic displacement parameters (IDPs) were refined using the JANA2006 program.[7] All fractional occupations—including those for $Sr^{2+}$ and $Ce^{3+}$—were at first allowed to vary and, after initial convergence, were subsequently constrained to the stoichiometric values. The thermal parameters for $Sr^{2+}$ and $Ce^{3+}$ were constrained to vary together equally.

## Results and Discussion

Grains of $Sr_{0.4}Ce_{0.4}TiO_3$ samples sintered at 1400 °C were far less defective than those sintered at 1300 °C, as can be seen in Figure 1. Most of the strain contrast presumably caused by a nonequilibrium distribution of cations in Figure 1a has been eliminated in Figure 1b.

The samples analyzed by XRD (Figure 2) all appeared to be single-phase, essentially consisting of a solid solution of $SrTiO_3$ and $Ce_2Ti_3O_9$ in a 2:1 ratio. The $Ce_2Ti_3O_9$ compound has been variously reported as either an undistorted perovskite with $Pm\bar{3}m$ symmetry[21] or a doubled perovskite with $Pmmm$ symmetry.[22] The oxygen-deficient versions of this phase are also typically reported in orthorhombic settings. Although the XRD pattern of $Sr_{0.4}Ce_{0.4}TiO_3$ published previously[1] can be indexed according to a cubic unit cell similar to pure $SrTiO_3$, electron diffraction[7] showed it to have a lower symmetry based on tilting of oxygen octahedra. Figure 3 shows selected area electron diffraction patterns (SADPs) parallel to the pseudo-cubic directions [100], [110], and [111] in an $x = 0.4$ sample obtained in this work.

Although the [111] pattern can be indexed unambiguously according to a primitive simple cubic perovskite

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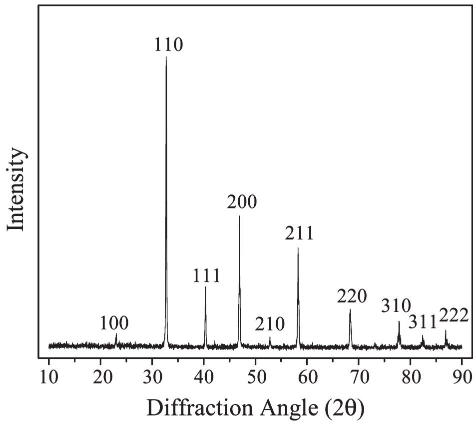

**Figure 2.** X-ray diffraction (XRD) pattern of $Sr_{0.4}Ce_{0.4}TiO_3$ at room temperature indexed according to a simple cubic perovskite unit cell.

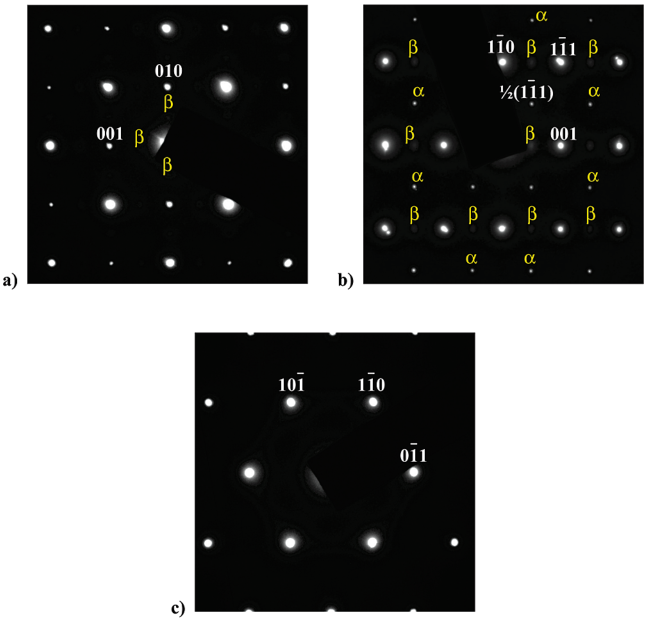

**Figure 3.** Selected-area electron diffraction patterns (SADPs) from grains of $Sr_{0.4}Ce_{0.4}TiO_3$ corresponding to the (a) [100], (b) [110], and (c) [111] pseudo-cubic directions. Superlattice reflections are denoted as either "α" or "*β*".

unit cell, the faint α superlattice reflections in the [110] pattern and even fainter *β* reflections in both the [100] and [110] cannot be explained by this structure. The α reflections in particular indicate that the lattice constant must be doubled and the symmetry lowered. The very weak and fuzzy nature of the *β* reflections indicates that they arise from a short-range ordering within the structure and not from true long-range periodicity. Even neglecting the *β* reflections, none of these patterns can be explained using Yoshii's $Ce_2Ti_3O_9$ model[22] in *Pmmm*. Ubic et al.[7] explained the structural distortion for $Sr_{1-3x/2}Ce_xTiO_3$ ($0.1333 \leq x \leq 0.25$) compositions as the result of antiphase octahedral tilting about the pseudo-cubic [111] (i.e., antiphase tilting of equal magnitude about each pseudo-cubic ⟨100⟩), resulting in a structure best described in space group $R\bar{3}c$. For this reason, it is unlikely that the structure of the $x = 0.4$ compound would contain tilts about just a single axis, as in the $I4/mcm$ model ($a^0a^0c^-$ tilt system) of $Sr_{1-3x/2}La_xTiO_3$ published by Howard et al.[5] In any event, some of the superlattice reflections observed here would be forbidden even by double diffraction in *I*4/*mcm*. The alternative *Cmmm* symmetry, also reported for $Sr_{1-3x/2}La_xTiO_3$ by Howard et al.,[5] allows tilting about two axes, but it would also allow {110} reflections here, which are never observed. Given the tilt system of the $0.1333 \leq x \leq 0.25$ compositions, the most likely distortion for $x = 0.4$ would involve antiphase tilts of *unequal* magnitude about the pseudo-cubic ⟨100⟩.

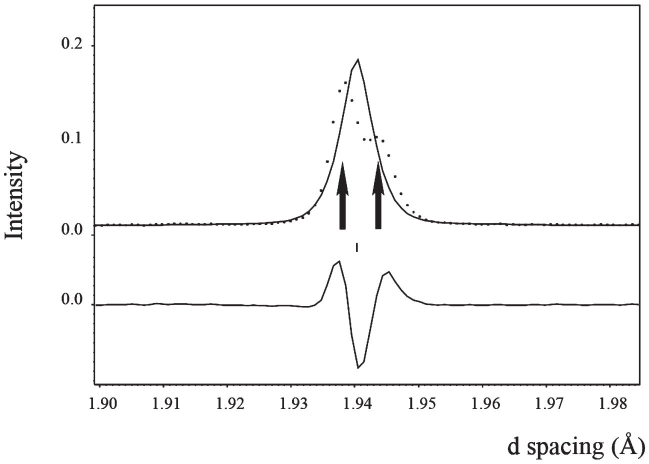

**Figure 4.** Peak splitting in neutron diffraction data of the (2$\bar{2}$4) reflection of $Sr_{0.4}Ce_{0.4}TiO_3$ modeled in $R\bar{3}c$.

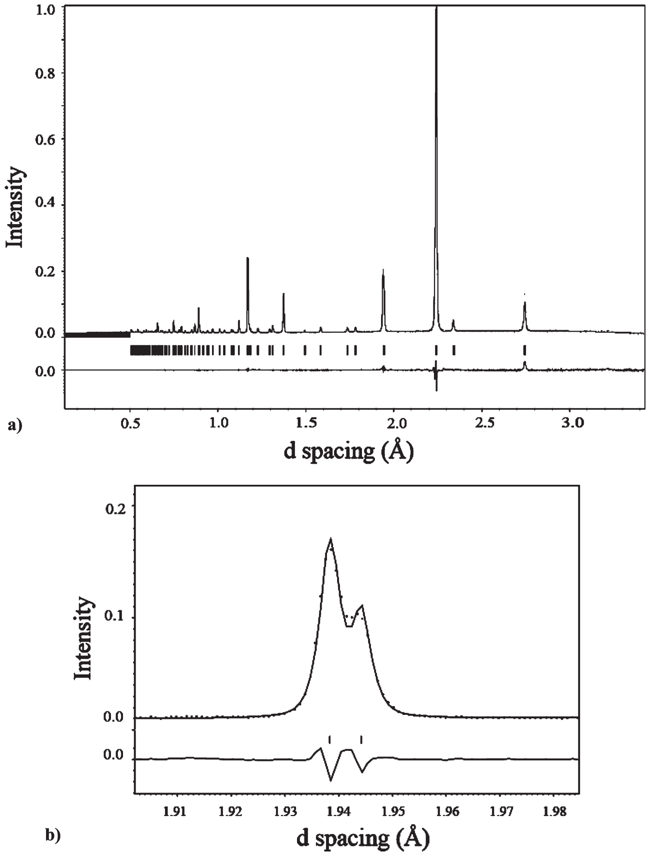

**Figure 5.** Refinement of neutron diffraction data in *C*2/*c* for $Sr_{0.4}Ce_{0.4}TiO_3$: (a) full pattern of bank 3 (115° bank) data and (b) a section that corresponds to that in Figure 4.

**Table 1. Refined Structural Parameters for $Sr_{0.4}Ce_{0.4}TiO_3$ at Room Temperature**[a]

| species | Wyckoff[b] | $x$ | $y$ | $z$ | SOF | $U_{iso/eq}$ (Å$^2$) |
|---|---|---|---|---|---|---|
| $Sr^{2+}$ | 4e | 0.5 | 0.2526 | 0.75 | 0.2667 | 0.0088(8) |
| $Ce^{3+}$ | 4e | 0.5 | 0.2526 | 0.75 | 0.2667 | 0.0088(8) |
| $Ti^{4+}$ | 4c | 0.25 | 0.25 | 0 | 0.6667 | 0.00913(8) |
| $O^{2-}$(1) | 8f | 0.754 | 0.5164 | 0.73 | 0.6667 | 0.0159(6) |
| $O^{2-}$(2) | 4e | 0.5 | 0.742 | 0.75 | 0.6667 | 0.0173(10) |

| species | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| $Sr^{2+}$ | 0.0095(4) | 0.0041(9) | 0.0123(10) | 0 | 0.0061(9) | 0 |
| $Ce^{3+}$ | 0.0095(4) | 0.0041(9) | 0.0123(10) | 0 | 0.0061(9) | 0 |
| $Ti^{4+}$ | 0.00913(8) | 0.00913(8) | 0.00913(8) | 0 | 0 | 0 |
| $O^{2-}$(1) | 0.0212(4) | 0.0165(7) | 0.0153(7) | −0.0035(9) | 0.0136(6) | −0.0089(6) |
| $O^{2-}$(2) | 0.0047(3) | 0.0245(15) | 0.0156(13) | 0 | 0.0018(10) | 0 |

[a] Estimated standard deviations are given in parentheses. [b] Space group $C2/c$ (No. 15), $a$ = 9.5228(3) Å, $b$ = 5.4869(2) Å, $c$ = 5.4818(2) Å, $\beta$ = 125.22(2)°, $V$ = 233.9(5) Å$^3$.

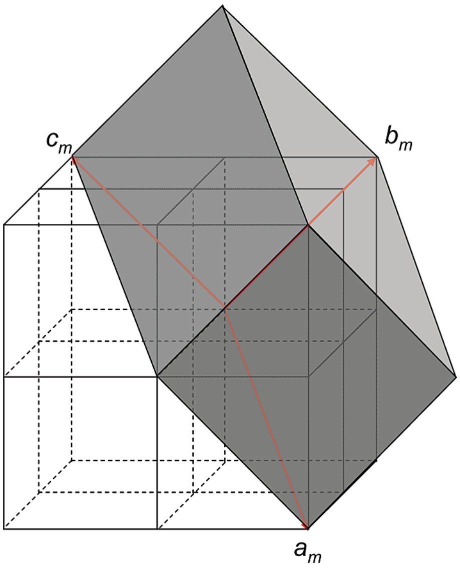

**Figure 6.** Geometrical relationship between the doubled cubic perovskite unit cell and the monoclinic unit cell.

The less-defective nature of samples sintered at 1400 °C in this work aided structural refinements of neutron diffraction data, which were used to refine the unit cell parameters, atomic positions, and isotropic displacement parameters (IDPs) for $Sr_{0.4}Ce_{0.4}TiO_3$. Background coefficients, scale factors, profile functions, and sample absorption were also refined for a total of 17 parameters.

Initial Rietveld refinements yielded satisfactory results in space group $R\overline{3}c$; however, for banks 3 and 4 (the two banks with the best resolution), the GOFs increase to 5−7 and there are some remaining residues in the difference curve. There is clearly a doubling (splitting) of some peaks associated with a lower symmetry (see Figure 4).

The *Cmmm* space group resulted in a better fit; however, this symmetry only explains the doubling of the peak at 1.95 Å and not the additional weak peak at ∼1.9 Å. Using the *Cmmm* space group, the refinement converges to $a$ = 7.7574(2) Å, $b$ = 7.7760(2) Å, and $c$ = 7.7501(2) Å. Such symmetry implies four different Sr/Ce mixed sites (0,0,0; $^1/_2$,0,0; $^1/_2$,0,$^1/_2$; 0,0,$^1/_2$), which could indicate an ordering between these two species, as reported by Howard et al.[5] for $Sr_{1-3x/2}La_xTiO_3$; however, ordering was not refined using the metric of this unit cell.

Three subgroups of $R\overline{3}c$ were also tested, including $C2/c$ and the noncentrosymmetric $C2$ and $Cc$. All three structural models yielded results better than for *Cmmm*, but both $C2$ and $Cc$ require many more parameters to refine than $C2/c$ and neither results in a significantly better fit. In addition, dielectric properties of $Sr_{0.4}Ce_{0.4}TiO_3$ do not suggest piezoelectricity. Indeed, all compositions within $Sr_{1-3x/2}Ce_xTiO_3$ ($0.154 \leq x \leq 0.4$) have recently been reported as incipient ferroelectrics;[17] therefore, the most probable structure is $C2/c$. The final refinement is demonstrated in Figure 5, and the atomic coordinates are shown in Table 1. The overall GOF is 2.94, $R_p$ = 5.14, and $R_{wp}$ = 3.64. As demonstrated in Figure 5b, the subtle splitting of peaks is fully accommodated within this model. Based on previous X-ray photoelectron spectroscopy (XPS) work,[1] the proportion of cerium present as $Ce^{4+}$ in these samples is likely to be < 5%, which is almost certainly compensated for by the reduction of ∼2% of the $Ti^{4+}$ to $Ti^{3+}$, neither of which should have a significant bearing on either electron diffraction or neutron diffraction results. A diagram of the geometrical relationship between the doubled cubic perovskite and the monoclinic unit cell is shown in Figure 6.

The lower symmetry is not due to cation ordering, which is not possible in $C2/c$, but rather purely oxygen displacements associated with distortion of the $TiO_6$ octahedra (see Figure 7). Octahedra appear to be tilted ∼4.7° about the $[100]_c$ but only ∼1.8° about the $[010]_c$ and $[001]_c$, corresponding to an $a^-b^-b^-$ tilt system, as anticipated. Compared to the structure of $Sr_{0.625}Ce_{0.25}TiO_3$ ($x$ = 0.25) refined previously[7] in $R\overline{3}c$, which showed octahedral tilting of ∼2° about all $\langle 100 \rangle_c$, $Sr_{0.4}Ce_{0.4}TiO_3$ ($x$ = 0.4) shows a much larger degree of tilt about the $[100]_c$ but virtually identical tilts about both the $[010]_c$ and $[001]_c$.

Figure 8 shows schematics of the same patterns in Figure 2 but indexed according to the monoclinic unit cell in $C2/c$. The extremely faint $\beta$ superlattice reflections visible in Figure 3 never coalesce into discrete spots and are probably the result of very short-range ordering phenomena. They might be explained by a very subtle and local doubling of the $c$-axis, as in the case of $BiCrO_3$,[23] still in space group $C2/c$. Alternatively, they may be related to the

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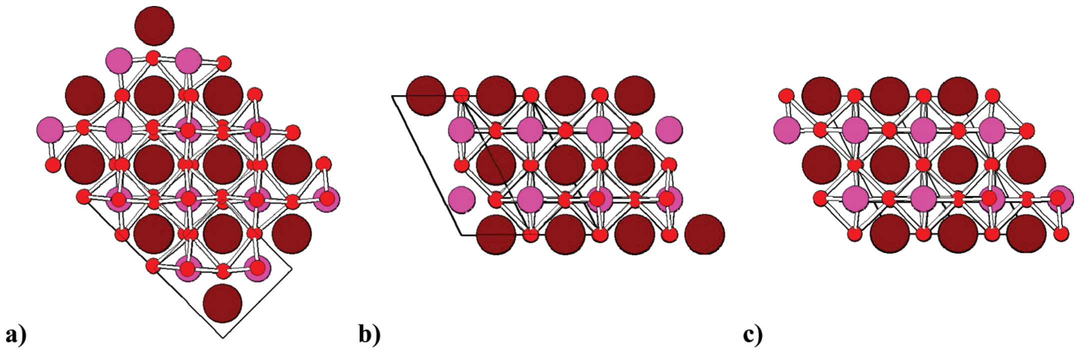

**Figure 7.** Projections of the $Sr_{0.4}Ce_{0.4}TiO_3$ crystal structure in $C2/c$ parallel to the three pseudo-cubic ⟨100⟩ (a) $[100]_c \| [101]_m$, (b) $[010]_c \| [01\bar{1}]_m$, and (c) $[001]_c \| [011]_m$. An outline of the monoclinic unit cell is superimposed in each case.

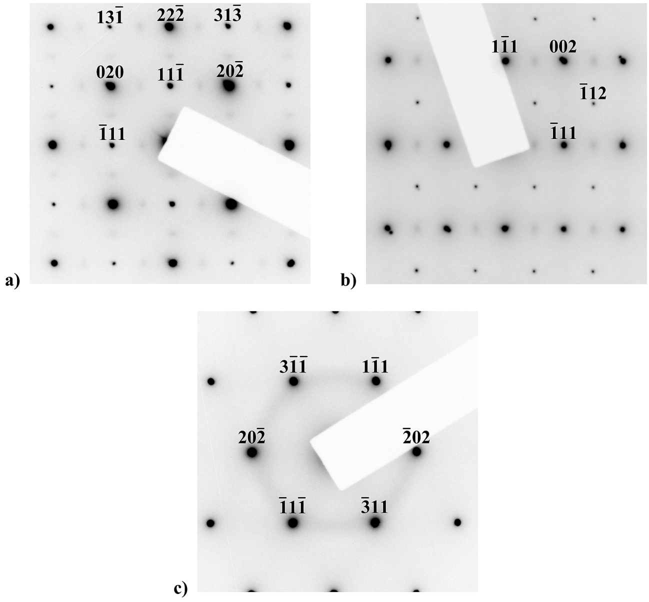

**Figure 8.** Schematic electron diffraction patterns corresponding to those in Figure 2 but indexed according to the monoclinic unit cell in $C2/c$ illustrated in Figure 6 parallel to (a) [101], (b) [110], and (c) [121].

incipient-ferroelectric nature of $Sr_{0.4}Ce_{0.4}TiO_3$. This doubling was not apparent or considered in the average structure refined from neutron diffraction data.

The refined pseudo-cubic lattice constant for this model is $a_c$ = 3.8819 Å. According to the formula developed by Ubic et al.,[19] which accounts for the effects of A-site cation vacancies, this value corresponds to a tolerance factor of $t$ = 0.9977. The model of Reaney et al.[24] for niobates and tantalates would predict an untilted structure for such high values of $t$. On the other hand, many researchers have reported structures of aluminates,[10] cuprates,[15] nickelates,[9] ferrites,[25] and titanates[7] with $t \approx 1$, which are stabilized by highly charged A-site cations and small tilt angles.

The average bond valence sums for the A, B, and O sites in $Sr_{0.4}Ce_{0.4}TiO_3$ are 2.0207, 4.2259, and 2.1637, respectively. These values are all in good agreement with those for both pure $SrTiO_3$ (2.1159, 4.1466, and 2.0875) as well as other $Sr_{1-3x/2}Ce_xTiO_3$ ($x < 0.4$) compounds,[7] which showed a general increase in bond valence sums with increasing cerium content. The increase in the A-site bond valence can be understood as a result of the combination of the partial substitution of $Ce^{3+}$ (1.34 Å) for $Sr^{2+}$ (1.44 Å), reducing the average A−O bond length, as well as the tendency of increasing tilts to reduce the cuboctahedral volume. The resulting smaller unit cell also reduces the average B−O bond lengths and so acts to increase the B-site bond valence.

## Conclusions

The perovskite compound $Sr_{0.4}Ce_{0.4}TiO_3$ has been produced in a phase-pure form and characterized crystallographically. Both electron diffraction and neutron diffraction show evidence of a noncubic supercell caused by antiphase tilting of oxygen octahedra. The superstructure is of a lower symmetry than for other $Sr_{1-3x/2}Ce_xTiO_3$ ($x < 0.4$) compositions; and the most likely space group is $C2/c$, corresponding to an $a^-b^-b^-$ tilt system. Octahedra are tilted by ∼4.7° about the pseudo-cubic $a$-axis and ∼1.8° about the pseudo-cubic $b$- and $c$-axes.

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**Supporting Information Available:** Crystallographic details of $Sr_{0.4}Ce_{0.4}TiO_3$ in the form of a CIF have been submitted. (CIF) This information is available free of charge via the Internet at http://pubs.acs.org/.

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