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Structure and Disorder in Single-Crystal Lead Zirconate, $PbZrO_3$

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Abstract

The full three-dimensional *single-crystal* crystal structure of the perovskite material $PbZrO_3$ (M_r = 346.42) has been refined. It is found that the structure is disordered with two substructure components related by a shear of $c/2$. Each individual substructure corresponds closely to the tilt system $a^-a^-c^o$ of Glazer [*Acta Cryst.* (1972), **B28**, 3384–3392; *Acta Cryst.* (1975), **A31**, 756–762]. The space group was determined to be *Pbam* (D^9_{2h}) with $a = 5.889$ (3), $b = 11.784$ (4) and $c = 8.226$ (2) Å, $V = 570.8$ (4) Å^3, $Z = 8$, $D_x = 8.06$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0.71069$ Å, $\mu = 612.68$ cm^{-1}, $T = 297$ K. The structure was refined to $R = 0.0596$ and $wR = 0.0753$ for 246 unique reflections, and, apart from the choice of space group, is very similar to that proposed by Whatmore (PhD thesis, Univ. of Cambridge, England, 1976). Comments are made on the relationship between the single-crystal structure of $PbZrO_3$ and that determined from polycrystalline samples.

Introduction

The perovskite compound $PbZrO_3$ has been of interest for some time because of the complex nature of its structure and also because it is the end member of the technologically important solid-solution series $PbZr_{1-x}Ti_xO_3$. For a long time there has been some controversy in the literature as to whether this material is ferroelectric or antiferroelectric. Roberts (1951) found evidence of piezoelectricity, thus pointing to a non-centrosymmetric space group. However, to observe this effect Roberts polarized a ceramic disc by applying a d.c. or pulsed electric field while cooling through the phase transition from 523 to 373 K. Given the well known problem of space charges in this material and taking into account the manner in which the sample was polarized, together with the very small effect found, suggests that this piezoelectric effect was probably due to an electret state induced by thermal charging, rather than to the symmetry of the crystal structure. It is not surprising, therefore, that others (*e.g.* Fesenko & Smotrakov, 1976; Scott & Burns, 1972) were unable to find polar effects although the occurrence of complex twinning in their crystals may have made such measurements suspect.

The crystal structure was first proposed by Sawaguchi, Maniwa & Hoshino (1951), who showed from weak X-ray superlattice reflections that the pseudocubic perovskite unit cell was given by $4\mathbf{a}_p \times 4\mathbf{b}_p \times 2\mathbf{c}_p$, with $\mathbf{a}_p = \mathbf{b}_p$. The quadrupling of the pseudocubic $\mathbf{a}_p$ and $\mathbf{b}_p$ axes could be explained by Pb displacements from their prototypic perovskite sites, as shown in Fig. 1. Sawaguchi *et al.* (1951) determined that the displacements were approximately 0.2 Å, and that the true space group was either *Pbam* or *Pba*2 with cell dimensions $\mathbf{a}_o = 5.87$, $\mathbf{b}_o = 11.74$ and $\mathbf{c}_o = 8.20$ Å. They were unable to locate the positions of the Zr or O ions, or to detect any displacements of the Pb ions out of the $(001)_o$ planes. Jona, Shirane, Mazzi & Pepinsky (1957) made a more detailed study of the structure using a combination of X-ray single-crystal and neutron powder diffraction. They found that the space groups that satisfied the systematic absence conditions were *Pbam* (D^9_{2h}), *Pba*2 (C^8_{2v}), *Pbnm* (D^{16}_{2h}) and *Pbn*2$_1$ (C^9_{2v}). Although they located the positions of the Zr and O ions to some extent, because they were unable to measure any reflections with l_o odd, they could not determine if the cations were displaced out of the $(001)_o$ planes. It was established that the oxygens formed octahedra that were approximately tilted with respect to the pseudocubic axes in the system $a^-a^-c^o$ of Glazer (1972, 1975). At the same time the octahedra were found to be greatly distorted, thus making identification of the tilt system difficult. Such large distortions are unusual in perovskites, except where large Jahn–Teller effects can occur, as in $KCuF_3$ (Okazaki & Suemune, 1961): this cannot be the case here. We therefore have reason to be concerned about the accuracy of the structure determination of Jona *et al.* (1957). It should be realized that their study only used projections to determine the structure and that, apart from Whatmore (1976) (see below), no full three-dimensional single-crystal structure determination has been published before now.

More recently, the structure of $PbZrO_3$ has been looked at again using powder neutron profile analysis (Sawaguchi, Shiozaki, Fujishita & Tanaka, 1980; Fujishita & Sawaguchi, 1981; Fujishita, Shiozaki, Achiwa & Sawaguchi, 1982; Fujishita & Hoshino, 1984). These authors found a better reliability factor for space group *Pbam* than for *Pba*2. Following this, Tanaka, Saito & Tsuzuki (1982*a*,*b*) claimed to determine the space group to be *Pbam* and to locate the oxygen coordinates using electron diffraction techniques.

In all of these structural studies, it was assumed that the structure was fully ordered, but it does not seem that the possibility of disorder has been considered to account for the apparently large octahedral distortions and the difficulty in determining the true structure of $PbZrO_3$. However, Whatmore (1976), in his PhD thesis, described an X-ray single-crystal structure refinement. Since this work was never published, we describe here the essential results of this work. Only one very small crystal of $PbZrO_3$ was found after an extensive attempt at crystal growth. Whatmore observed the *only* systematic absences to be *h*00 for *h* odd, 0*k*0 for *k* odd and 00*l* for *l* odd, consistent with space groups $P2_12_12_1$, $P2_12_12$, $P2_122_1$, $P22_12_1$, $P2_122$, $P22_12$, $P222_1$ and $P222$. Furthermore, he pointed out that the observation of reflections of the type 102, 012, 032 and 018 ruled out both space groups *Pbam* and *Pba*2. By assuming that the original structure determination of Sawaguchi *et al.* (1951) and Jona *et al.* (1957) was essentially correct, Whatmore determined that the only possible space groups were $P2_12_12_1$ and $P2_12_12$. With either space group, difference maps revealed elongated or split densities at the oxygen positions, indicative of structural disorder. He showed that the structure could be considered to be the superposition of two $PbZrO_3$ structures, each of which had significantly less octahedral distortion than in previous work. Subsequently he found that $P2_12_12$ (D^3_2) gave the best fit to the data. On the other hand, using neutron powder Rietveld refinement, Whatmore redetermined the structure to be fully ordered. By comparison with the disordered X-ray structure, he found that the neutron powder structure was very similar to one of the two superposed structures making up the disordered structure. This raises the intriguing possibility that the structure of crystallites in a powder prepared by firing mixed oxides might be different from that of a single crystal. It is possible that the original crystal was twinned and that this would explain the apparent disorder. We therefore felt that a new single-crystal structure determination could resolve the confusion in this material.

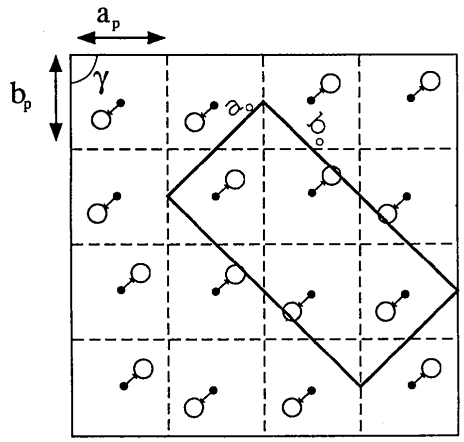

Fig. 1. Schematic diagram showing Pb displacements in $PbZrO_3$ as viewed on (001). Both pseudocubic and conventional unit cells are displayed.

Crystal growth

Single crystals were obtained by the flux method from 77 mol% PbO, 20.6 mol% B_2O_3 and 2.4 mol% $PbZrO_3$. A mixture of previously synthesized $PbZrO_3$ was placed for 4 h in a Pt–Ir crucible with a constant temperature gradient along the axis of the crucible of 10 K cm^{-1}, maintaining the bottom at 1373 K. Then the gradient was reduced to 8 K cm^{-1} and the melt was cooled at a rate of 8 K h^{-1}. At a temperature of about 1173 K the solution was poured out and, after the solution has been cooled to ambient temperature, the crystals were washed in an aqueous solution of acetic acid. Transparent, light-grey and homogeneous crystals in the form of thin rectangular plates were obtained. Optical and dielectric tests showed only one phase transition from the paraelectric to antiferroelectric state.

Thermo-optical examination carried out under a polarizing microscope showed that the 513 K phase transition in the crystals is accompanied by formation of phase boundaries with a prominent crystallographic plane {310} (Dec, 1989; Dec & Kwapuliński, 1989). In order to obtain a monodomain state, it was necessary to pass through the phase transition with a single phase boundary. This was done in a special furnace in which the temperature gradient was almost perpendicular (± 5 K) to the required phase boundary. Under these conditions uniform cooling of the crystal through the phase transition point led to an entirely monodomain state (Fig. 2).

Experimental

A small crystal measuring 0.07 × 0.07 × 0.03 mm was cut out of a larger single-domain slice. Under a polarizing microscope, this crystal appeared still to be single-domain. X-ray measurements were made on a Stoe Stadi-4 diffractometer with graphite-monochromated Mo $K\alpha$ radiation. The peak shapes of several trial reflections were found to be well defined. The intensity data were collected between $2\theta = 3$ and 65° for two equivalent regions, assuming orthorhombic symmetry, as well as their Friedel equivalents. 2892 reflections were measured in total (2588 with l even and 304 with l odd). Three intensity control reflections were monitored hourly and every 2 h, the orientation matrix was remeasured using 30 reflections. No systematic deviations in the check reflections were observed, and the average variation was less than 2%. The intensities were consistent with orthorhombic symmetry and on the basis of this the lattice parameters were measured by the double step-scanning procedure (scanning both sides of the $2\theta = 0°$ position) applied to 18 reflections. After refinement, with the axes restricted to be orthogonal, the lattice parameters were found to be $a = 5.889$ (3), $b = 11.784$ (4) and $c = 8.226$ (2) Å. In order to correct for the effects of absorption 18 reflections were measured by ψ scans. The data were corrected for Lp factors and for absorption with the Stoe programme *EMPIR* followed by *REDU*4 to produce a structure factor list: $\mu R = 2.1$ (min. and max. transmission factors were 0.0122 and 0.0902, respectively). On merging with the program *CRYSTALS*, $R_{\rm int} = 0.082$ based on 2548 reflections, giving a unique set of 637 reflections. 36 reflections had structure factors less than $3\sigma(F)$ and were removed, as well as 344 systematically absent reflections.

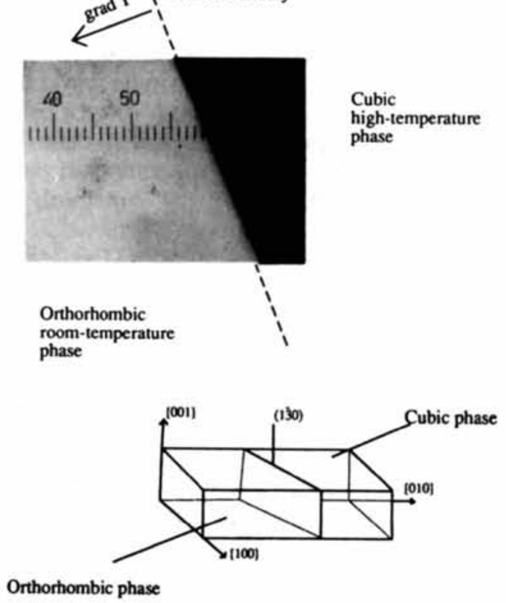

Fig. 2. Sharp phase boundary seen between crossed-polars in a temperature gradient of 10 K mm^{-1}. 1 division = 10 μm. The indices marked in the figure are with reference to the pseudo-cubic axes.

The systematic absences at the level of $3\sigma(I)$ were of the form $0kl$ ($k = 2n + 1$) and $h0l$ ($h = 2n + 1$). In addition, there were no reflections of the type odd–0–odd, suggesting that there is no need to invoke an n-glide perpendicular to b. Thus the likely space group, given earlier considerations, is either *Pbam* (D_{2h}^9) or *Pba*2 (C_{2v}^8). A careful search for reflections 102, 012, 032 and 018 failed to reveal any intensity and so we can discount the space group $P2_12_12$ (D_2^3) (note that this is a maximal subgroup of *Pbam*) used by Whatmore. A possible reason for this difference may be that Whatmore grew his crystal out of a melt containing a small amount of TiO_2.

As a starting model we used the fractional coordinates of Pb and Zr found by Whatmore, modified to take account of the different choice of space group with Pb on mirror planes perpendicular to c:

		x	y	z
Pb1	4(g)	0.703	0.124	0
Pb2	4(h)	0.708	0.130	$\frac{1}{2}$
Zr	8(i)	0.240	0.130	0.250

Refinement of 246 of $|F(hkl)| > 3\sigma$ was carried out with *CRYSTALS*, incorporating neutral atomic scattering factors and anomalous-scattering factors taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). After a few cycles of full-matrix refinement, with weights proportional to $1/\sigma(F_{\rm obs})$ including isotropic temperature factors and the extinction factor, difference Fourier maps were calculated in order to locate the oxygens. Fig. 3 shows Fourier difference sections in particular regions where oxygens were expected. It is immediately noticeable that most of the oxygen density appears to be split into pairs (only O5 does not appear to show significant splitting). This turns out to be almost exactly the same as that observed by Whatmore in his thesis, and so confirms the suggestion of substantial disorder (either thermal or static) in this crystal. The positions of the oxygens were then added to the model and several cycles of refinement were carried out on the positions and anisotropic temperature factors of Pb and Zr as well as on the isotropic temperature factors for the oxygens (these were restrained to refine together) and the extinction and scale factors. The final agreement was $R = 0.0596$ and $wR = 0.0753$. Table 1 lists the final atomic coordinates and temperature factors.* Refinement in space group *Pba*2 gave no further improvement, and so, as far as our measurements are concerned, we may consider the structure to be centrosymmetric *Pbam*.

Discussion of the structure

From Table 1 it is found that the cation displacements from the ideal perovskite positions are very similar to those found in earlier work, and so deserve no comment. What is new is the evidence of splitting of oxygen peaks (the splitting is 0.69 Å for O1, 0.86 Å for O2, 0.68 Å for O3 and 0.81 Å for O4) pointing to disorder in the structure. It is possible by examination of the bond lengths to separate the observed average structure into two component substructures (Figs. 4 and 5). The relationship between the substructures almost exactly corresponds to a displacement through $(0,0,\frac{1}{2})$ thus:

$$x_A, y_A, z_A \rightarrow x_B, y_B, \tfrac{1}{2} + z_B. \qquad (1)$$

With reference to pseudocubic perovskite axes, it can be seen from Fig. 4 in particular that the tilting of the octahedra in each substructure is well described by the tilt scheme $a^-a^-c^0$ of Glazer (1972, 1975).† In fact each substructure conforms rather better to this tilt system than could be seen in the earlier structure determinations published for $PbZrO_3$. Moreover, we see that the sense of tilts in the *A* substructure is almost exactly reversed in the *B* substructure. Table 2 lists the O—O distances in an octahedron for each substructure. The average O—O distance is almost the same in each case, 2.98 Å, with a spread of about 0.2 Å representing the octahedral distortion. As a better measure of the similarity of the two substructures we calculate the average of the modulus of the differences between bond lengths related by the displacement relationship (1) to be 0.03 (3) Å *i.e.* zero to within one standard deviation. Thus substructures *A* and *B* can be taken to be identical. It is important to stress that we cannot differentiate for certain between static and dynamic disorder here, although it seems that the large displacements between the oxygens of the *A* substructure and the *B* substructure would be more suggestive of a static disorder model.

We must address the question as to whether the split oxygen peaks are really a feature of disorder in the single-crystal structure or an artifact of some

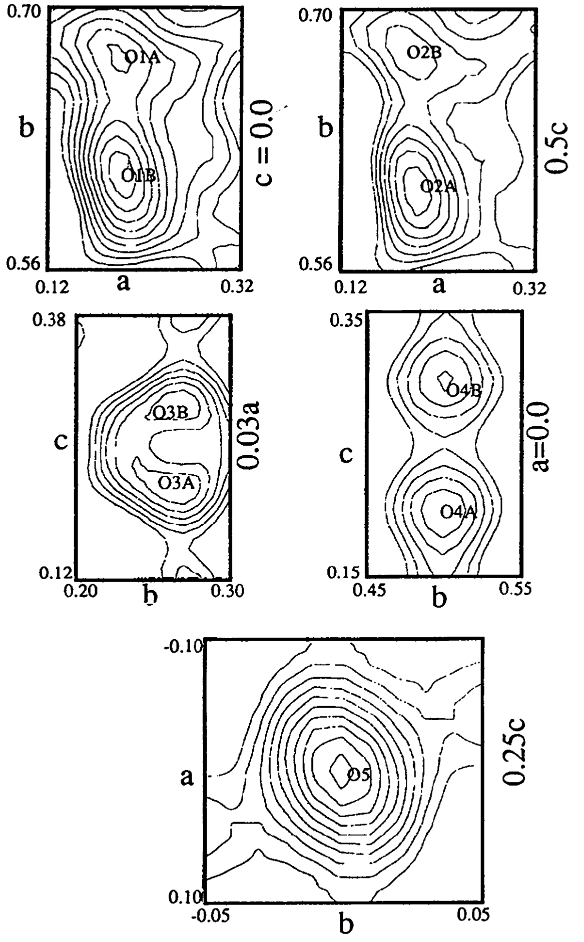

Fig. 3. Fourier difference maps of the oxygen positions in $PbZrO_3$.

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* Lists of structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71145 (7 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HU0418]

† A crystal with this tilt system alone would have the space group *Imam* (D_{2h}^{28}) (Glazer, 1972, 1975). The cation displacements and resulting distortions of the octahedra arise through the group–subgroup relationship

$$Imam \rightarrow Pmam \xrightarrow{2\times b} Pbam.$$

Pmam does not occur in practice since b_o is doubled by the antiparallel shifts of the Pb atoms.

Table 1. *Fractional coordinates and thermal parameters with e.s.d.'s in parentheses*

$T = \exp[-2\pi^2(U_{11}h^2a^{*2} + \ldots + 2U_{12}hka^*b^* + \ldots)]$, where U_{ij} are in Å^2. For oxygens, the isotropic U is given (all restrained to be equivalent).

	Site	Point symmetry	Occupancy	x	y	z
Pb1	4(*g*)	..*m*	1.00	0.705 (4)	0.124 (2)	0
Pb2	4(*h*)	..*m*	1.00	0.711 (5)	0.131 (2)	0.5
Zr	8(*i*)	1	1.00	0.2435 (7)	0.132 (3)	0.25 (3)
O1*A*	4(*g*)	..*m*	0.50	0.3083	0.1720	0
O1*B*	4(*g*)	..*m*	0.50	0.3057	0.1132	0
O2*A*	4(*h*)	..*m*	0.50	0.2993	0.1044	0.5
O2*B*	4(*h*)	..*m*	0.50	0.3103	0.1770	0.5
O3*A*	8(*i*)	1	0.50	0.0316	0.2666	0.2914
O3*B*	8(*i*)	1	0.50	0.0292	0.2651	0.2089
O4*A*	4(*f*)	..2	0.50	0	0.50	0.1993
O4*B*	4(*f*)	..2	0.50	0	0.50	0.2980
O5	4(*e*)	..2	1.00	0	0	0.2507

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pb1	0.012 (5)	0.043 (7)	0.021 (7)	0	0	−0.010 (5)
Pb2	0.027 (6)	0.010 (4)	0.018 (6)	0	0	0.014 (4)
Zr	0.008 (2)	0.012 (6)	0.009 (6)	−0.004 (9)	0.000 (9)	0.004 (2)
O1*A*	0.034 (8)					
O1*B*	0.034 (8)					
O2*A*	0.034 (8)					
O2*B*	0.034 (8)					
O3*A*	0.034 (8)					
O3*B*	0.034 (8)					
O4*A*	0.034 (8)					
O4*B*	0.034 (8)					
O5	0.034 (8)					

type of twinning. Certainly, no twins were observed on a macroscopic scale under a polarizing microscope and, so if present, were likely to be of a size below the optical coherence length. Now, the observed relationship (1) between the *A* and *B* substructures, namely a shift of *c*/2, suggests that the domains are related by a simple slip or shear of *nc*/2 (*n* odd). If these domains are larger than the X-ray coherence length, there will be no effect on the diffraction intensities, and hence on the observed positions of the atoms in the structure determination, since the two substructures are simply related by a shift of origin. The fact that we observe split peaks then *necessitates* that any domains of this type must be smaller than the X-ray coherence length, and so amount to a form of disorder as far as structure determination is concerned. It is also worth recording that X-ray measurements on a second crystal gave precisely the same apparent disorder. The fact that equal amounts of *A* and *B* substructures were found in both crystals studied by us, as well as in the crystal studied by Whatmore, again suggests that the *A* and *B* domains are probably very small but great in number. As no extra reflections or diffuse scattering were observed, we must consider the domains to be randomly, or near randomly, distributed.

Shear domains in $PbZrO_3$ have been commented on by Tanaka, Saito & Tsuzuki (1982*a*,*b*) and by Prisedskii, Komarov, Panko, Dobrikov & Klimov (1979) and Dobrikov & Presnyakova (1981). The shear boundaries observed by the Japanese group involved shifts in the structure that resulted in domains of a few tens of Å in size in which they suggest the pattern of Pb displacements is disturbed. If this were the case in our crystal, we should have expected to find split Pb peaks. Our proposed shear domains, however, involve only disturbances to the oxygen framework. Fig. 6 illustrates how we may envisage the slip boundary in our case. Note that, because the Pb displacements are identical in columns down the *c* axis, the slip along *c*/2 does not change the Pb displacements: indeed the fact that along *c* the displacements of the Pb atoms lie along planes *c*/2 apart provides a natural stimulus to maintaining any slip to be through *nc*/2 (*n* odd) increments. Our picture of the local disorder is similar to the well known crystallographic shear structures (see for example, Hyde & Andersson, 1989). In this case, the shear does not lead to a new structure but to a disordered form. In order to allow such a shear to take place, we have to allow for local oxygen vacancies to provide broken bonds.

Such a picture can be used to explain the observation by Whatmore that the structure determination by powder diffraction shows just a single structure. It has been established that the behaviour of $PbZrO_3$ is considerably altered by defects (*e.g.* see Roleder & Dec, 1989). The crystal used in our study was cut from a larger crystal that showed the behaviour normally expected of a relatively defect-free crystal. The powders are normally made by firing of mixed oxides in the solid state, whereas the crystals are

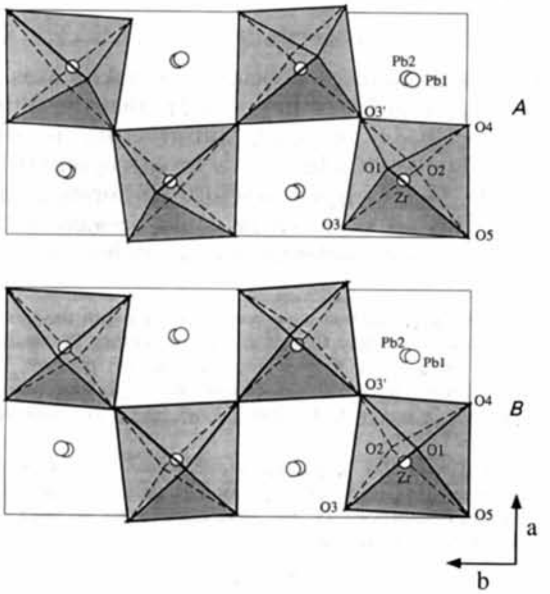

Fig. 4. The structure of $PbZrO_3$ on (001) divided into its two constituent substructures *A* and *B*.

grown out of high-temperature solution. In fact, these two technological processes differ and lead to different stoichiometries of the samples. The low solubility of $PbZrO_3$ determines the chemical composition of the starting melt which contains a large amount of PbO. Thus the crystal growth takes place in an environment with a PbO excess. Under these conditions a crystal with an excess of PbO may be produced in which there are vacancies in the Zr and O sites ($Pb^{2+}Zr^{4+}_{1-x}O^{2-}_{3-2x}$ or $Pb^{2+}_{1-4x}Pb^{3+}_{4x}Zr^{4+}_{1-x}O^{2-}_3$) or with Pb^{4+} ions replacing Zr^{4+} ($Pb^{2+}Pb^{4+}_xZr^{4+}_{1-x}$-$O^{2-}_3$ – no vacancies) (Haertling & Land, 1971; Wojcik & Ujma, 1989). It should be pointed out that in each case there are no vacancies in the Pb sites. For ceramic samples, firing of a stoichiometric mixture of oxides lasting many hours gives rise to both Pb and O vacancies, because of the volatility of PbO at high temperature ($Pb_{1-x}ZrO_{3-x}$). Hence, the different stoichiometries of the crystals and ceramics lead to different internal stains and this is probably the main reason for the appearance or presence of shear disorder in the $PbZrO_3$ structure. Moreover, crystal growth happens more rapidly and so is in less of an equilibrium: in this case the shears will form on a fine scale and in large numbers to make an effectively equal concentration of the two substructures throughout the crystal bulk. During ceramic manufacture the controlling factor is the diffusion rates of the various constituents, which are quite slow, thus allowing for the strain that would normally be encountered due to defect creation to be minimized. If our model is correct, then a structure determination of a crystal that has been so treated as to contain little or no oxygen defects should not show the disorder found here. Experiments are in progress to verify if this is so.

Table 2. *Bond lengths* (Å) *for the oxygens in the octahedra*

Substructure *A*		Substructure *B*		|Δ| (Å)
O1—O3	3.106	3.091	O2—O3	0.015
O1—O3′	2.828	2.804	O2—O3′	0.024
O1—O4	2.841	2.891	O2—O4	0.050
O1—O5	3.414	3.449	O2—O5	0.035
O2—O3	3.014	2.968	O1—O3	0.046
O2—O3′	2.670	2.597	O1—O3′	0.073
O2—O4	3.005	3.016	O1—O4	0.011
O2—O5	2.971	3.045	O1—O5	0.074
O3—O3′	2.970	2.966	O3—O3′	0.004
O3′—O4	2.859	2.869	O3′—O4	0.010
O4—O5	2.975	2.970	O4—O5	0.005
O5—O3	3.165	3.148	O5—O3	0.017
			Mean |Δ|	0.03 (3)

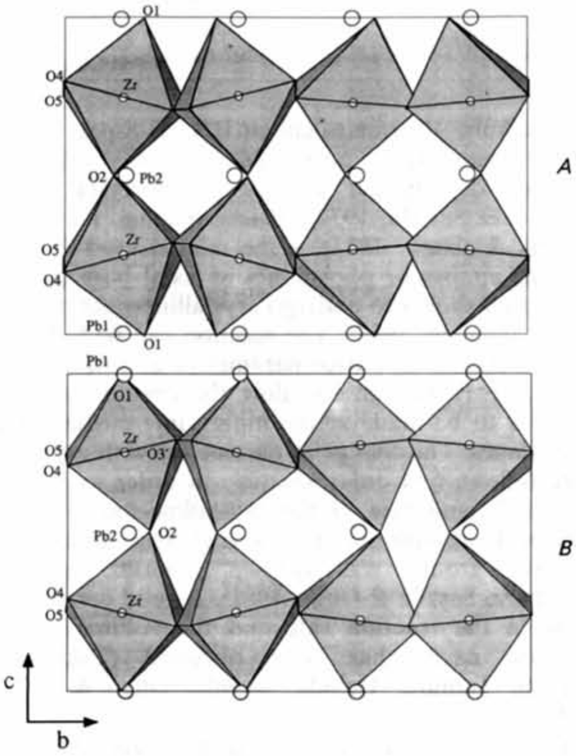

Fig. 5. The structure of $PbZrO_3$ on (100) divided into its two constituent substructures *A* and *B*.

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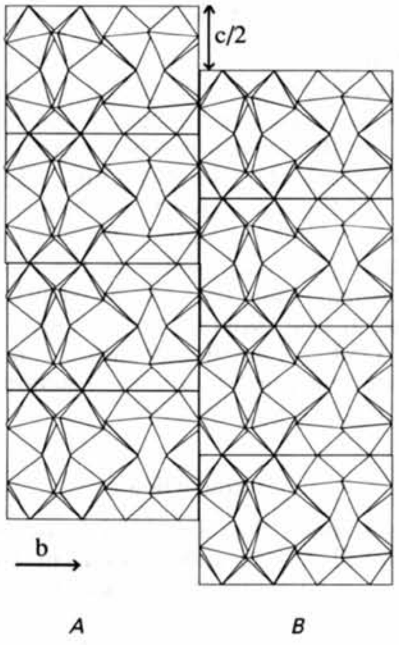

Fig. 6. A schematic view of how substructures *A* and *B* can be joined together to form a shear of *c*/2.

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Crystalline-State Reaction of Cobaloxime Complexes. 16.[*] Two Polymorphs of [(*S*)-1-Cyanoethyl][(*S*)-phenylethylamine]cobaloxime

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Abstract

Two polymorphs were found for the title complex. One is racemized without degradation of the crystallinity on exposure to visible light as well as X-rays, whereas the other, which has two solvent molecules in an asymmetric unit, is non-reactive. The different reactivities of two crystal forms can be well explained by the size of the reaction cavity for the chiral 1-cyanoethyl group. The rates of the racemization were measured and the crystal structures were determined at four different temperatures, 223, 253, 296 and 333 K. A good correlation was obtained between the rate constant and the reaction cavity in the range of these temperatures.

Introduction

Since it was found that the chiral 1-cyanoethyl (ce) group bonded to the cobalt atom in the crystal of [(*R*)-1-cyanoethyl][(*S*)-phenylethylamine]bis(2,3-butanedione dioximato)cobalt(III), *R*-*S*-pea cobaloxime complex, is racemized by X-ray exposure without degradation of the single-crystal form (Ohashi & Sasada, 1977; Ohashi, Yanagi, Kurihara, Sasada & Ohgo, 1981), some related crystals with various amines or phosphines as axial base ligands have been shown to undergo crystalline-state racemization (Ohashi, 1988). The reaction can be followed by the change in lattice parameters and often proceeds slowly enough to allow the crystal structure analysis to be made at the initial, intermediate and final stages. The change in parameters with exposure time follows first-order kinetics. In order to explain the mode and rate of the crystalline-state racemization, the reaction cavity, the void space around the reactive group, was defined (Ohashi, Yanagi, Kurihara, Sasada & Ohgo, 1981). A good correlation between the reaction rate and the volume of the reaction cavity has been obtained (Takenaka, Ohashi, Tamura, Uchida, Sasada, Ohgo & Baba, 1993).

Recently, the complex of [(*S*)-1-cyanoethyl][(*S*)-phenylethylamine]cobaloxime, *S*-*S*-pea, which is a diastereoisomer of *R*-*S*-pea, was found to have two

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[*] Part 15: Osano, Danno, Uchida, Ohashi, Ohgo & Baba (1991).

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