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SHORT COMMUNICATIONS

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On the dualistic interpretation of the symmetry of the incommensurately modulated structure of NbTe₄. By SANDER VAN SMAALEN, *Laboratory of Inorganic Chemistry, Materials Science Centre, University of Groningen, Nijenborgh 16, 9747 AG Groningen, The Netherlands*

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Abstract

The dualistic interpretation of the symmetry of the incommensurately modulated structure of NbTe₄ is considered. It is shown that the previously determined structure is in full accordance with this description of the symmetry.

The symmetry of incommensurately modulated structures can be described by the so-called superspace groups (de Wolff, Janssen & Janner, 1981). Then, for each independent modulation wave vector an additional coordinate is defined, and the symmetry operations are given by 3-d reducible matrices operating in a (3+d)-dimensional space.

De Wolff (1984) has developed an alternative description in which the symmetry of the basic structure and the modulation are given by separate three-dimensional space groups. It was shown that for one-dimensional modulations this dualistic description and the superspace-group approach are equivalent, whereas for higher-dimensional modulations, the dualistic description is the less general one (de Wolff, 1984).

Recently, Prodan & Boswell (1987) have applied the dualistic interpretation of the symmetry to the incommensurately modulated phase of NbTe₄. One of their conclusions was that the structure of NbTe₄ as determined from X-ray diffraction by van Smaalen, Bronsema & Mahy (1986)* is not in accordance with the dualistic description of the symmetry. This would mean that the symmetry restrictions derived for the modulation functions are already in error. In this note it will be shown that the previously determined structure exhibits the full dualistic symmetry.

From X-ray diffraction the (3+1)-dimensional superspace group was determined as $W_{111}^{P4/mcc}$ with modulation wave vector $\mathbf{q} = (\frac{1}{2}, \frac{1}{2}, 0.691)$ (van Smaalen *et al.*, 1986). In the dualistic approach, two 3D space groups have to be specified, one for the basic structure and one for the modulation wave. For NbTe₄ they are $G_B = P4/mcc$ and $G_M = I4/mmm$, respectively (Prodan & Boswell, 1987).

In Fig. 1 a projection of the basic structure on the *ab* plane is given. As defined by van Smaalen *et al.* (1986), we will use the larger unit cell $A \times B \times C$ ($C = c$), in which the modulation wave vector has only one irrational component: $\mathbf{q}_i = (0, 0, 0.691)$. In order to explain the different symmetry operators, the two atoms denoted by 1 and 2 will be considered in more detail.

In the basic structure these two atoms are related by a *c*-glide plane perpendicular to *A*. In the superspace group the symmetry operation between those two atoms is $\left\{ \begin{smallmatrix} 1 \\ 1 \end{smallmatrix} \right\}$.

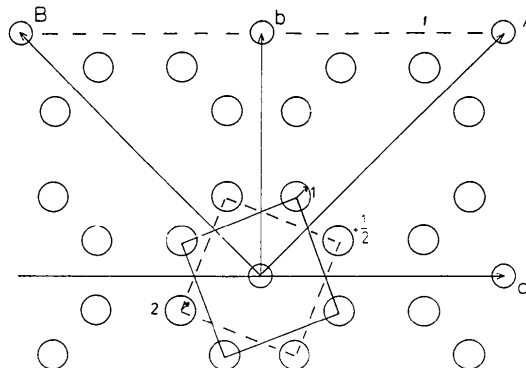


Fig. 1. Projection of the basic structure. Large circles denote Te atoms, small circles denote Nb atoms. Shown are the original (*a, b*) unit cell and the transformed (*A, B*) cell. The atoms indicated by 1 and 2 correspond to those in Fig. 2.

* Fig. 4 of van Smaalen *et al.* (1986) contains some errors. B_{1z} for Nb in Table 8 should be $-0.03899(2)$, in accordance with the values given in Table 7.

For the x component of the modulation function this means that if $u_x^1 = u_x(\mathbf{q}_i \cdot \mathbf{r}_1^0)$, then $u_x^2 = -u_x(\mathbf{q}_i \cdot \mathbf{r}_2^0)$, with $\mathbf{r}_1^0 = (x, y, 0)$ and $\mathbf{r}_2^0 = (-x, y, \frac{1}{2})$.

In the dualistic description the symmetry is split into two parts. The first is G_B , which gives the symmetry of the basic structure. Atoms 1 and 2 are related by a c glide, c_x . The second is G_M , which gives the symmetry of the modulation pattern. The key point of the dualistic interpretation is that G_M defines the symmetry of the modulation functions considered as continuous functions in space. In general,

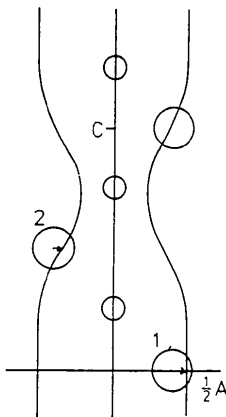


Fig. 2. Projection on the AC plane (see Fig. 1). The wavy lines describe the modulation functions of atoms 1 and 2, respectively. The amplitude is exaggerated by a factor of five.

this symmetry does not apply to the displacements of the two atoms related by an element of G_B . Therefore, to test for the presence of a mirror plane in G_M , we have to compare the values of \mathbf{u}^1 and \mathbf{u}^2 at the corresponding positions. Substitution of the components of \mathbf{q}_i and of $\mathbf{r}_1^0 = (x, y, z)$ and $\mathbf{r}_2^0 = (-x, y, z)$ into the above expressions for \mathbf{u}^1 and \mathbf{u}^2 , immediately shows the presence of a mirror plane as symmetry element of the modulation pattern. In Fig. 2 the relationship between average positions, atomic displacements and the modulation pattern is illustrated. A similar analysis for the other atoms and the other symmetry elements shows that the structure as determined by van Smaalen *et al.* (1986) has the full G_M symmetry.

In conclusion, we have shown that, contrary to the assertion of Prodan & Boswell (1987), the previously determined modulated structure of NbTe_4 (van Smaalen *et al.*, 1986) is in full accordance with the dualistic interpretation of the symmetry of this compound.

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Preliminary X-ray studies of adult δ -crystallin: evidence of a space-group transition. By S. E. MYLVAGANAM, C. SLINGSBY, P. F. LINDLEY* and T. L. BLUNDELL, *Laboratory of Molecular Biology, Department of Crystallography, Birkbeck College (University of London), Malet St., London WC1E 7HX, England*

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Abstract

A new calcium-dependent crystal form of δ -crystallin grown at ambient temperatures using vapour-diffusion methods exhibits a temperature-dependent space-group transition. At lower temperatures the crystal form adopts space group $P2_12_12$ with $Z=2$ and exhibits a diffraction pattern corresponding to the crystal form reported previously, while at 294 K the resulting space group is $P2_12_12_1$ in which the c axis doubles to $140.2(2) \text{ \AA}$ with $Z=4$. A third crystal form which requires a higher concentration of calcium ions shows no such transition and appears to be remarkably stable to X-rays in comparison with the other crystal forms. These crystals diffract to at least 2.4 \AA in space group $P2_12_12_1$ with $Z=4$ and have the largest cell dimensions of the three crystal forms with $a = 88.9(1)$, $b = 144.8(1)$ and $c = 152.5(1) \text{ \AA}$.

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Introduction

Previous X-ray studies on crystals of the avian eye lens tetrameric protein, δ -crystallin (200kd), from adult turkey, showed that variations in the c dimension (of up to 22%) were dependent on the hydration level of the crystal, and furthermore, that such dramatic changes had little effect on crystal symmetry (Narebor & Slingsby, 1985). We present here further X-ray studies on three crystal forms of δ -crystallin grown either in the absence or in the presence of calcium ions.

Experimental

Crystal form I was grown at 277 K using $0.05 M$ sodium acetate buffer, pH 4.3, and crystallization conditions described by Narebor, Slingsby, Lindley & Blundell (1980). For crystal forms II and III, which were grown at ambient temperature [294(1) K], sodium acetate buffer was