

Precise Structure Analysis by Neutron Diffraction for $R\text{NbO}_4$ and Distortion of NbO_4 Tetrahedra

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Abstract

Precise crystal structure analysis by neutron powder diffraction is performed for rare-earth orthoniobates ($R\text{NbO}_4$: $R = \text{La, Nd, Ho}$ and Yb) and the distortion of NbO_4 tetrahedra is estimated with the normal-coordinate method. Displacement of the cubic symmetry mode is large and increases with decreasing ionic radius of $^{\text{VIII}}R^{3+}$. This displacement produces a regular tetrahedron of NbO_4 . The mean value of Nb-O distances in the regular tetrahedron of $R\text{NbO}_4$ crystals is 1.834 Å. This value is nearly equal to the mean bond length for $s=5/4$, $\bar{R}=1.828$ Å, estimated by the bond-valence method. Displacements of the other symmetry modes slightly decrease or are almost constant with decreasing ionic radius.

1. Introduction

There are several reports on the structural study of rare-earth orthoniobate ($R\text{NbO}_4$) crystals by X-ray diffraction (Brixner, Whitney, Zumsteg & Jones, 1977; Tsunekawa & Takei, 1978; Mariathasan, Finger & Hazen, 1985) and neutron diffraction (David, 1983; David, Hull & Ibberson, 1990). The low-temperature symmetry was determined by convergent-beam electron diffraction and found to be space group $C2/c$ ($=I2/a=I2/c$) (Tanaka, Saito & Watanabe, 1980).

The characteristic behavior of NbO_4 tetrahedra in LaNbO_4 has been studied by high-pressure X-ray diffraction (Mariathasan, Finger & Hazen, 1985) and

neutron diffraction (David, Hull & Ibberson, 1990). It was shown in terms of bond-valence concepts (Brown & Wu, 1976) that the coordination number of Nb^{5+} ions tends to change from four to six as the ferroelastic transition temperature is approached from higher temperatures. The effect of hydrostatic pressure on the transition temperature was explained by the same tendency.

We have investigated pseudoelasticity (rubber-like behavior) in LaNbO_4 and NdNbO_4 crystals. It was suggested that the role of NbO_4 tetrahedra, which have twofold symmetry (monoclinic deformation), is very important (Tsunekawa, Suezawa & Takei, 1977).

In this paper we report the precise structure analysis by neutron powder diffraction of $R\text{NbO}_4$ crystals ($R = \text{La, Nd, Ho}$ and Yb) and describe the distortion of NbO_4 tetrahedra with the normal-coordinate method.

2. Experimental

Powder samples were prepared by crushing and grinding single crystals grown by the Czochralski or floating-zone method. Neutron powder diffraction data were taken at room temperature using the high-resolution TOF (time-of-flight) neutron powder diffractometer (HRP) ($\Delta d/d \approx 3 \times 10^{-3}$) installed at the KENS pulsed-spallation neutron source at the National Laboratory for High Energy Physics (Watanabe, Asano, Iwasa, Satoh, Murata, Karahashi, Tomiyoshi, Izumi & Inoue, 1987). These data were refined with a TOF neutron diffraction version of

the *RIETAN* program (Izumi, Asano, Murata & Watanabe, 1987).

3. Results

All Rietveld refinement patterns of the HRP data for $R\text{NbO}_4$ ($R = \text{La}, \text{Nd}, \text{Ho}$ and Yb) show a good fit. An example is shown in Fig. 1. Final R factors, lattice constants and structural parameters with their standard deviations are listed in Table 1, where R_{wp} became smaller than R_e for NdNbO_4 and HoNbO_4 because the fit is quite good and the background is relatively high. In Table 1, the temperature factor of Nb in HoNbO_4 was assigned to be isotropic because U_{11} became slightly negative in an anisotropic assignment. Niobium-oxygen interatomic distances and angles calculated with the *ORFFE* program (Busing, Martin & Levy, 1964) are given in Table 2.

4. Discussion

The NbO_4 tetrahedra in $R\text{NbO}_4$ crystals have monoclinic deformation. Such a deformation is decomposed into 12 normal modes (Kataoka, 1991) as shown in Fig. 2. The displacement of these modes, Q_n , is estimated by the normal-coordinate method, where the subscripts $n = 1, 2, 3, \dots, 11$ and 12 correspond to a cubic mode, an orthorhombic mode, a tetragonal mode, three monoclinic symmetry modes, three translational modes and three rotational modes, respectively.

$$Q_1 = [1/(12)^{1/2}] [(q_{1x} - q_{1y} + q_{1z}) + (-q_{2x} + q_{2y} + q_{2z}) + (q_{3x} + q_{3y} - q_{3z}) - (q_{4x} + q_{4y} + q_{4z})] \quad (1a)$$

$$Q_2 = (1/8^{1/2}) [(q_{1x} + q_{1y}) - (q_{2x} + q_{2y}) + (q_{3x} - q_{3y}) - (q_{4x} - q_{4y})] \quad (1b)$$

$$Q_3 = (1/4) [(2q_{1z} - q_{1x} + q_{1y}) + (2q_{2z} + q_{2x} - q_{2y}) - (2q_{3z} + q_{3x} + q_{3y}) - (2q_{4z} - q_{4x} - q_{4y})] \quad (1c)$$

$$Q_4 = (1/8^{1/2}) [(q_{1y} - q_{1z}) + (q_{2y} + q_{2z}) - (q_{3y} - q_{3z}) - (q_{4y} + q_{4z})] \quad (1d)$$

$$Q_5 = (1/8^{1/2}) [(q_{1x} + q_{1z}) + (q_{2x} - q_{2z}) - (q_{3x} - q_{3z}) - (q_{4x} + q_{4z})] \quad (1e)$$

$$Q_6 = (1/8^{1/2}) [(-q_{1x} + q_{1y}) + (q_{2x} - q_{2y}) + (q_{3x} + q_{3y}) - (q_{4x} + q_{4y})] \quad (1f)$$

$$Q_7 = (1/2)(q_{1x} + q_{2x} + q_{3x} + q_{4x}) \quad (1g)$$

$$Q_8 = (1/2)(q_{1y} + q_{2y} + q_{3y} + q_{4y}) \quad (1h)$$

$$Q_9 = (1/2)(q_{1z} + q_{2z} + q_{3z} + q_{4z}) \quad (1i)$$

$$Q_{10} = (1/8^{1/2}) [-(q_{1y} + q_{1z}) - (q_{2y} - q_{2z}) + (q_{3y} + q_{3z}) + (q_{4y} - q_{4z})] \quad (1j)$$

$$Q_{11} = (1/8^{1/2}) [(q_{1x} - q_{1z}) + (q_{2x} + q_{2z}) - (q_{3x} + q_{3z}) - (q_{4x} - q_{4z})] \quad (1k)$$

$$Q_{12} = (1/8^{1/2}) [(q_{1x} + q_{1y}) - (q_{2x} + q_{2y}) - (q_{3x} - q_{3y}) + (q_{4x} - q_{4y})]. \quad (1l)$$

Therefore, we can get the values of Q_n , substituting the values of q_{ix} , q_{iy} and q_{iz} ($i = 1, 2, 3$ and 4) that correspond to x , y and z coordinates of O atoms

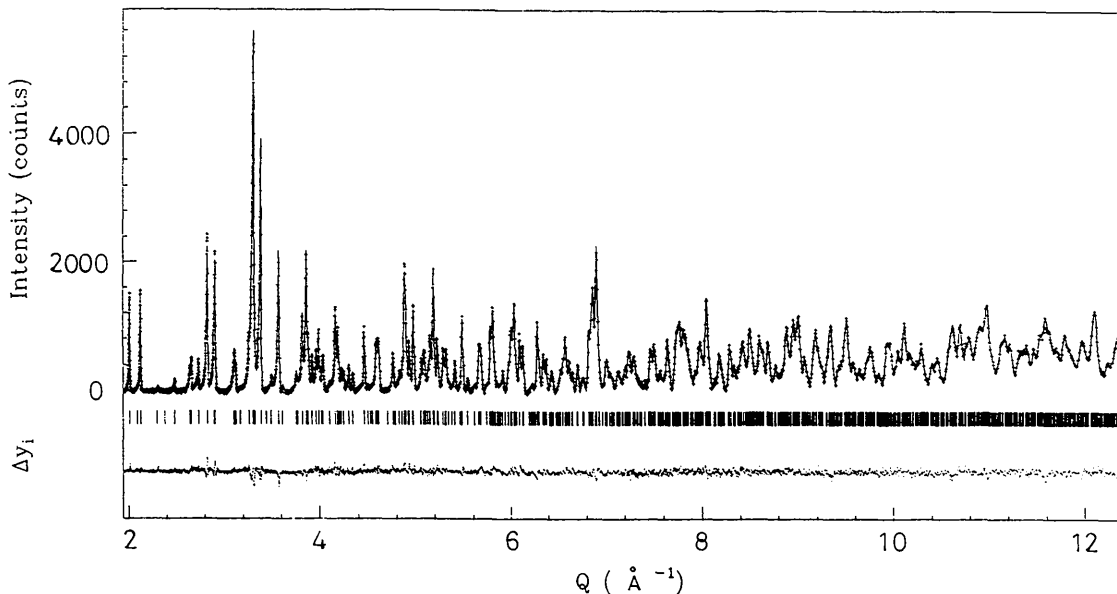


Fig. 1. Rietveld refinement pattern of the HRP data for HoNbO_4 . $Q = 2\pi/d$, where d is the interplanar spacing, and $\Delta y_i = y_i(o) - y_i(c)$, where $y_i(o)$ is the observed intensity and $y_i(c)$ is the calculated intensity at a particular channel i .

Table 1. *Structural parameters for RNbO₄ (R = La, Nd, Ho and Yb) at room temperature*

The R factors R_{wp} and R_p are defined for all the data points in a profile with and without a weight. R_i and R_f are for the integrated Bragg intensity and the structure factor. R_e is an expected R factor. Lattice parameters in the brackets were obtained by Aldred (1984). g is the occupation factor.

(a) LaNbO₄ ($I2/a=I2/c$), $R_{wp}=4.45$, $R_p=3.42$, $R_e=3.72$, $R_i=3.01$, $R_f=1.63\%$; $a=5.5647$ (1), $b=11.5194$ (2), $c=5.2015$ (1) Å, $\beta=94.100$ (1) $^\circ$ [$a=5.5667$ (2), $b=11.5245$ (4), $c=5.2020$ (3) Å, $\beta=94.084$ (2) $^\circ$]

Atom	Site	g	x	y	z	U_{11} (Å ²)	U_{22} (Å ²)	U_{33} (Å ²)	U_{12} (Å ²)	U_{13} (Å ²)	U_{23} (Å ²)	B_{eq} (Å ²)
La	4(e)	1	0	0.6292 (1)	1/4	0.0052 (5)	0.0007 (5)	0.0058 (5)	0	0.0028 (4)	0	0.30
Nb	4(e)	1	0	0.1036 (1)	1/4	0.0018 (6)	0.0024 (6)	0.0049 (7)	0	0.0005 (5)	0	0.24
O(1)	8(f)	1	0.2376 (2)	0.0337 (1)	0.0546 (2)	0.0080 (6)	0.0042 (5)	0.0109 (7)	0.0007 (5)	0.0059 (5)	0.0011 (5)	0.60
O(2)	8(f)	1	0.1460 (2)	0.2042 (1)	0.4888 (2)	0.0063 (6)	0.0043 (5)	0.0066 (6)	0.0005 (5)	-0.0008 (4)	-0.0024 (5)	0.45

(b) NdNbO₄ ($I2/a=I2/c$), $R_{wp}=3.18$, $R_p=2.49$, $R_e=3.32$, $R_i=2.50$, $R_f=1.42\%$; $a=5.4669$ (1), $b=11.2789$ (2), $c=5.1463$ (1) Å, $\beta=94.503$ (1) $^\circ$ [$a=5.4687$ (3), $b=11.2811$ (5), $c=5.1466$ (3) Å, $\beta=94.528$ (4) $^\circ$]

Atom	Site	g	x	y	z	U_{11} (Å ²)	U_{22} (Å ²)	U_{33} (Å ²)	U_{12} (Å ²)	U_{13} (Å ²)	U_{23} (Å ²)	B_{eq} (Å ²)
Nd	4(e)	1	0	0.6296 (1)	1/4	0.0032 (3)	0.0037 (4)	0.0032 (3)	0	0.0015 (2)	0	0.26
Nb	4(e)	1	0	0.1040 (1)	1/4	0.0024 (4)	0.0051 (4)	0.0037 (4)	0	0.0008 (3)	0	0.30
O(1)	8(f)	1	0.2399 (2)	0.0327 (1)	0.0467 (2)	0.0068 (4)	0.0065 (4)	0.0077 (4)	0.0011 (3)	0.0035 (3)	0.0017 (3)	0.55
O(2)	8(f)	1	0.1508 (2)	0.2065 (1)	0.4907 (2)	0.0053 (4)	0.0076 (4)	0.0056 (4)	0.0003 (3)	-0.0009 (3)	-0.0032 (3)	0.49

(c) HoNbO₄ ($I2/a=I2/c$), $R_{wp}=3.06$, $R_p=2.42$, $R_e=3.18$, $R_i=2.71$, $R_f=1.19\%$; $a=5.2985$ (1), $b=10.9465$ (2), $c=5.0719$ (1) Å, $\beta=94.531$ (1) $^\circ$ [$a=5.3030$ (2), $b=10.9555$ (3), $c=5.0742$ (2), $\beta=94.548$ (3) $^\circ$]

Atom	Site	g	x	y	z	U_{11} (Å ²)	U_{22} (Å ²)	U_{33} (Å ²)	U_{12} (Å ²)	U_{13} (Å ²)	U_{23} (Å ²)	B_{eq} (Å ²)
Ho	4(e)	1	0	0.6288 (1)	1/4	0.0030 (4)	0.0009 (3)	0.0033 (3)	0	0.0016 (2)	0	0.19
Nb	4(e)	1	0	0.1061 (1)	1/4	0.0024 (4)	0.0051 (4)	0.0037 (4)	0	0.0008 (3)	0	0.12 (2)
O(1)	8(f)	1	0.2458 (2)	0.0324 (1)	0.0415 (2)	0.0057 (4)	0.0038 (4)	0.0049 (4)	0.0010 (3)	0.0017 (3)	0.0005 (3)	0.38
O(2)	8(f)	1	0.1566 (2)	0.2100 (1)	0.4971 (2)	0.0035 (4)	0.0039 (4)	0.0055 (4)	0.0005 (3)	-0.0015 (3)	-0.0018 (3)	0.34

(d) YbNbO₄ ($I2/a=I2/c$), $R_{wp}=4.04$, $R_p=3.15$, $R_e=3.18$, $R_i=3.25$, $R_f=1.37\%$; $a=5.2394$ (1), $b=10.8344$ (2), $c=5.0436$ (1) Å, $\beta=94.467$ (1) $^\circ$ [$a=5.2429$ (3), $b=10.843$ (1), $c=5.0456$ (3), $\beta=94.496$ (7) $^\circ$]

Atom	Site	g	x	y	z	U_{11} (Å ²)	U_{22} (Å ²)	U_{33} (Å ²)	U_{12} (Å ²)	U_{13} (Å ²)	U_{23} (Å ²)	B_{eq} (Å ²)
Yb	4(e)	1	0	0.6286 (1)	1/4	0.0015 (5)	0.0015 (4)	0.0031 (5)	0	0.0016 (4)	0	0.16
Nb	4(e)	1	0	0.1067 (2)	1/4	0.0013 (8)	0.0028 (8)	0.0011 (8)	0	0.0004 (6)	0	0.13
O(1)	8(f)	1	0.2473 (4)	0.0321 (2)	0.0401 (3)	0.0051 (6)	0.0041 (7)	0.0071 (8)	0.0016 (6)	0.0037 (6)	0.0015 (5)	0.42
O(2)	8(f)	1	0.1583 (3)	0.2106 (2)	0.4997 (3)	0.0032 (6)	0.0036 (7)	0.0054 (7)	0.0007 (5)	-0.0002 (5)	-0.0022 (5)	0.32

O(3), O(1), O(4) and O(2) into (1a) to (1l), where it is noted that the position of the Nb atom is taken as the origin and the coordinate system is not oblique but orthogonal, different from those in Table 1. We obtain:

$$Q_{1,La} = 3.6575 (2), \quad Q_{1,Nd} = 3.6714 (1) \quad (2a)$$

$$Q_{1,Ho} = 3.6744 (2), \quad Q_{1,Yb} = 3.6691 (3)$$

$$Q_{2,La} = -0.0950 (2), \quad Q_{2,Nd} = -0.1111 (1) \quad (2b)$$

$$Q_{2,Ho} = -0.1322 (2), \quad Q_{2,Yb} = -0.1429 (3)$$

$$Q_{3,La} = -0.2215 (2), \quad Q_{3,Nd} = -0.2391 (1) \quad (2c)$$

$$Q_{3,Ho} = -0.2658 (2), \quad Q_{3,Yb} = -0.2767 (3)$$

$$Q_4 = 0 \quad (2d)$$

$$Q_5 = 0 \quad (2e)$$

$$Q_{6,La} = -0.3155 (2), \quad Q_{6,Nd} = -0.3356 (1) \quad (2f)$$

$$Q_{6,Ho} = -0.3254 (2), \quad Q_{6,Yb} = -0.3163 (3)$$

$$Q_7 = 0 \quad (2g)$$

Table 2. *Bond lengths and angles of RNbO₄ (R = La, Nd, Ho and Yb), where the angles O(2)–Nb–O(3) and O(3)–Nb–O(4) are equal to O(1)–Nb–O(4) and O(1)–Nb–O(2), respectively, owing to twofold symmetry of the NbO₄ tetrahedron*

The notation O(1)–Nb–O(3) etc. is taken from Tsunekawa & Takei (1978).

	$A-B-C$	$A-B$ (Å)	$B-C$ (Å)	$A-B-C$ (°)
LaNbO ₄	O(1)–Nb–O(3)	1.903 (1)	1.903 (1)	129.9 (1)
	O(2)–Nb–O(4)	1.844 (1)	1.844 (1)	102.2 (1)
	O(1)–Nb–O(4)	1.903 (1)	1.844 (1)	109.65 (6)
	O(1)–Nb–O(2)	1.903 (1)	1.844 (1)	101.28 (6)
NdNbO ₄	O(1)–Nb–O(3)	1.918 (1)	1.918 (1)	130.36 (7)
	O(2)–Nb–O(4)	1.842 (1)	1.842 (1)	102.22 (7)
	O(1)–Nb–O(4)	1.918 (1)	1.842 (1)	109.96 (7)
	O(1)–Nb–O(2)	1.918 (1)	1.842 (1)	100.71 (4)
HoNbO ₄	O(1)–Nb–O(3)	1.919 (1)	1.919 (1)	130.31 (8)
	O(2)–Nb–O(4)	1.841 (1)	1.841 (1)	103.65 (8)
	O(1)–Nb–O(4)	1.919 (1)	1.841 (1)	110.23 (4)
	O(1)–Nb–O(2)	1.919 (1)	1.841 (1)	99.99 (4)
YbNbO ₄	O(1)–Nb–O(3)	1.915 (2)	1.915 (2)	130.1 (1)
	O(2)–Nb–O(4)	1.838 (2)	1.838 (2)	104.5 (1)
	O(1)–Nb–O(4)	1.915 (2)	1.838 (2)	110.42 (8)
	O(1)–Nb–O(2)	1.915 (2)	1.838 (2)	99.67 (7)

$$Q_8 = 0$$

$$Q_{9,\text{La}} = -0.3524 (2), \quad Q_{9,\text{Nd}} = -0.3519 (2)$$

$$Q_{9,\text{Ho}} = -0.3316 (2), \quad Q_{9,\text{Yb}} = -0.3175 (3)$$

$$Q_{10} = 0$$

$$Q_{11} = 0$$

$$Q_{12,\text{La}} = 0.6336 (2), \quad Q_{12,\text{Nd}} = 0.6070 (1)$$

$$Q_{12,\text{Ho}} = 0.6016 (2), \quad Q_{12,\text{Yb}} = 0.5986 (3)$$

where $Q_{n,\text{La}}$ is the displacement, in Å, of n th normal mode for LaNbO_4 crystals, and so on.

The displacement Q_1 produces a regular tetrahedron of NbO_4 . Four sets of orthogonal coordinates, q_{ix}^0 , q_{iy}^0 and q_{iz}^0 ($i = 1, 2, 3$ and 4), brought about by

(2h) only one mode of Q_1 , are estimated using an inverse transformation matrix:

(2i) $q_{1x}^0 = Q_1/(12)^{1/2}, \quad q_{1y}^0 = -Q_1/(12)^{1/2}$ and (3a)

(2j) $q_{1z}^0 = Q_1/(12)^{1/2};$

(2k) $q_{2x}^0 = -Q_1/(12)^{1/2}, \quad q_{2y}^0 = Q_1/(12)^{1/2}$ and (3b)

$$q_{2z}^0 = Q_1/(12)^{1/2};$$

(2l) $q_{3x}^0 = Q_1/(12)^{1/2}, \quad q_{3y}^0 = Q_1/(12)^{1/2}$ and (3c)

$$q_{3z}^0 = -Q_1/(12)^{1/2};$$

$q_{4x}^0 = -Q_1/(12)^{1/2}, \quad q_{4y}^0 = -Q_1/(12)^{1/2}$ and (3d)

$$q_{4z}^0 = -Q_1/(12)^{1/2}.$$

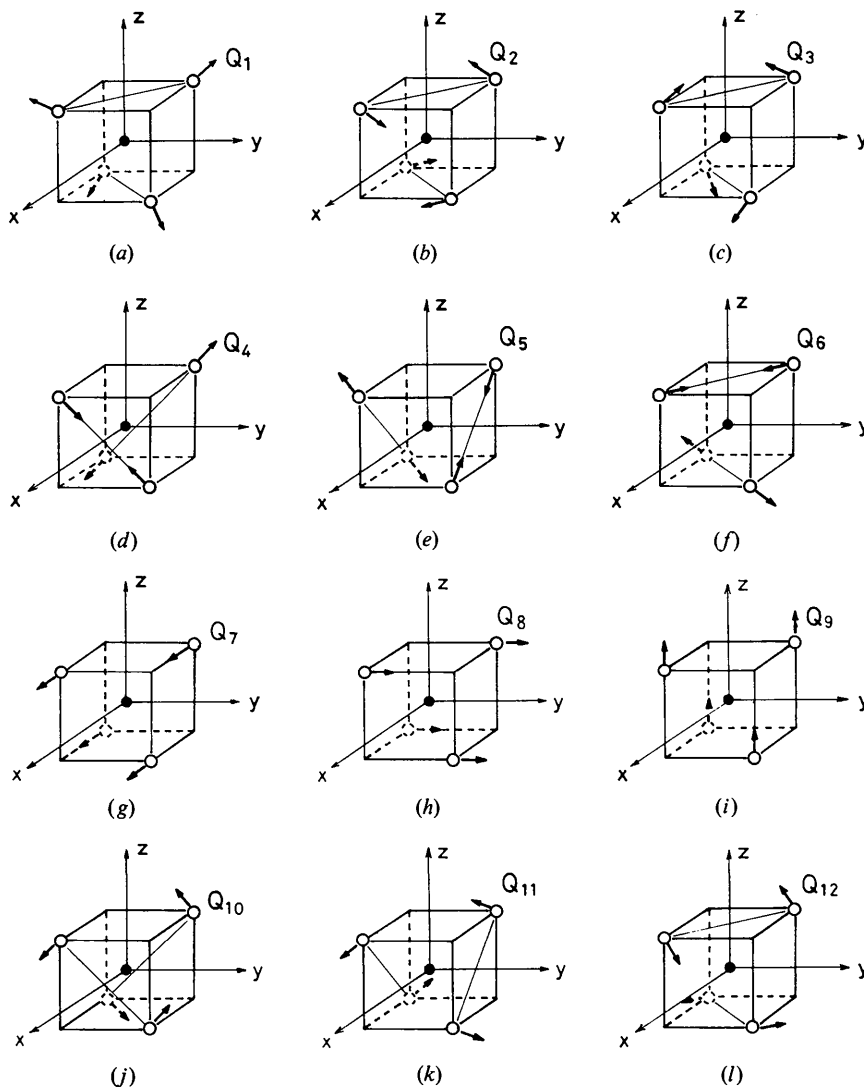


Fig. 2. Twelve normal modes for a distorted NbO_4 tetrahedron: one mode of (a) cubic, (b) orthorhombic and (c) tetragonal symmetries; (d) to (f) three modes of monoclinic symmetry; (g) to (i) three translational modes; and (j) to (l) three rotational modes. The displacements of these modes, Q_n , are shown by solid arrows. Open circles are O atoms and filled circles are Nb atoms.

These four sets correspond to the positions of four O atoms in the regular tetrahedron. Thus, the virtual bond length of Nb–O, ℓ_0 , is given by

$$\ell_0 = \{[Q_1/(12)^{1/2}]^2 + [-Q_1/(12)^{1/2}]^2 + [Q_1/(12)^{1/2}]^2\}^{1/2} = Q_1/2. \quad (4)$$

The mean value of Q_1 is 3.668 Å, from (2a), and so the average value of ℓ_0 is 1.834 Å. This value is nearly equal to the mean bond length $\bar{R}=1.828$ Å for s (= valence of Nb/coordination number of Nb) = 5/4, where s was called the electrostatic bond strength by Pauling (1929) and the bond valence by Brown (1978), $\bar{R} = R_0 - 0.37 \ln S$ and $R_0 = 1.911$ Å (Brown & Altermatt, 1985).

We can estimate a rate of displacement for each normal mode (a kind of distortion) by the following

equation:

$$\varepsilon_n = Q_n/V^{1/3} \quad (5)$$

where $V = abc \sin \beta$ is the monoclinic unit-cell volume of $R\text{NbO}_4$ and $n = 1, 2, 3, 6, 9$ and 12. Substituting each displacement value into (5), we get the results as shown in Fig. 3. It is noted that the rate of Q_1 displacement, ε_1 , increases with decreasing ionic radius of ${}^{\text{VIII}}R^{3+}$. On the other hand, the rates of displacement of other symmetry modes slightly decrease or are almost constant with decreasing ionic radius. The variations in the rates of these displacements towards lower temperatures for pseudoelasticity are considered to be important.

5. Concluding remarks

Our results are summarized as follows:

(1) Precise crystal data for $R\text{NbO}_4$ ($R = \text{La}, \text{Nd}, \text{Ho}$ and Yb) at room temperature were obtained by the high-resolution TOF neutron powder diffraction method.

(2) It was shown with the normal-coordinate method that the virtual bond length of the regular tetrahedron NbO_4 in $R\text{NbO}_4$ crystals is 1.834 Å on average, which is nearly equal to the mean bond length for an ideal bond valence of $s = 5/4$.

(3) The rate of displacement of each normal mode to cube root of the unit-cell volume was estimated. The relations between those rates and the ionic radii of rare-earth elements were obtained at room temperature.

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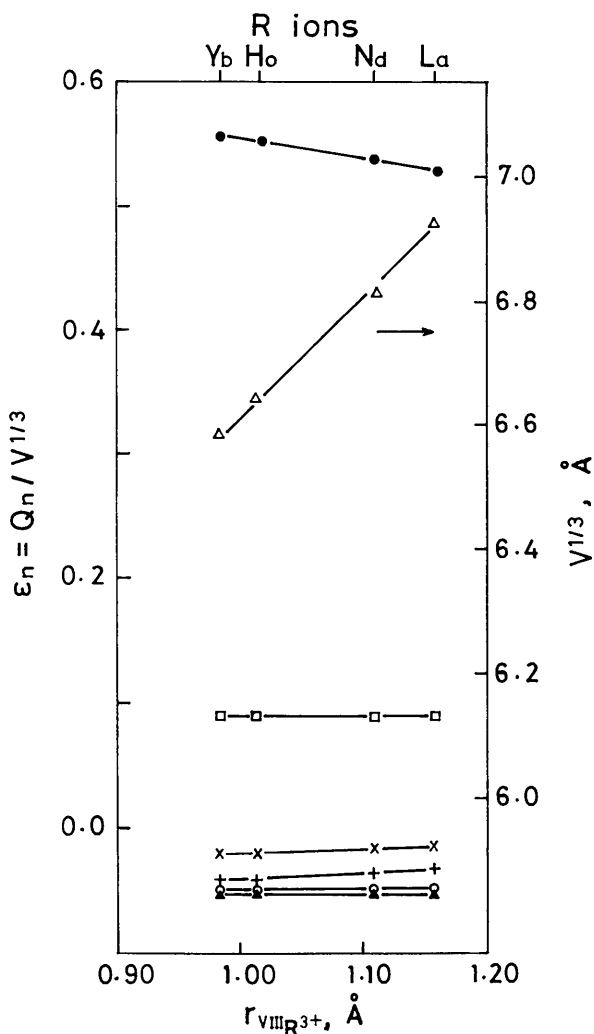


Fig. 3. Relation between the ionic radius of the rare-earth element (Shannon, 1976) and both the rate of displacement of each mode, ε_n , and $V^{1/3}$, where $n=1$ (●), $n=2$ (x), $n=3$ (+), $n=6$ (○), $n=9$ (▲), $n=12$ (□) and V is the unit-cell volume (Δ).

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Phase Determination of X-ray Reflections in a Quasicrystal

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Abstract

Multiple Bragg diffraction effects have been observed in an Al–Cu–Fe quasicrystal. The experimental data are analyzed by means of a multibeam perturbation theory. Good fits are obtained between experimental and calculated profiles. The feasibility for phase determination of structure factors is demonstrated. It is found that there is no inversion symmetry in Al–Cu–Fe.

1. Introduction

It has been shown recently that multiple Bragg scattering can be used for phase determination of X-ray structure factors (Shen & Colella, 1987). The general idea is to monitor the intensity of a weak reflection as the crystal is rotated around the scattering vector. When a strong reflection is excited simultaneously, the diffracted intensity exhibits a peak as a function of ψ , the azimuthal angle of rotation, with asymmetric side bands. It has been pointed out (Chapman, Yoder & Colella, 1981) that phase information can be obtained from the asymmetric side bands using n -beam dynamical theory, even when dealing with mosaic crystals of general shape (Shen & Colella, 1987).

A general review of multibeam literature was published a few years ago (Chang, 1987) and recently phase effects have been observed in protein crystals (Hümmer, Schwegle & Weckert, 1991; Chang, King, Huang & Gao, 1991).

In this paper we report the observation of multiple-diffraction (Renninger) effects in a quasicrystal. Since a quasicrystal does not possess long-range periodicity in the usual sense, it is not clear that all diffraction

features present in ordinary crystals should be visible in quasicrystals. However, we know that strong and sharp Bragg diffraction spots are produced by quasicrystals. We also know how to predict the positions of nodes in reciprocal space.* A necessary condition for the existence of the Renninger effect is that the difference between the Miller indices of two Bragg reflections must also correspond to a Bragg reflection. Since the xyz coordinates of every node in reciprocal space are expressed by means of a linear combination of six Miller indices, the necessary condition mentioned above is certainly satisfied in a quasicrystal.

2. Experimental

Since multiple-beam effects are more visible for weak reflections, we decided to concentrate on the reflection $240442 = \mathbf{P}$, which was chosen on the basis of a precession photograph taken perpendicularly to the fivefold axis. Bragg nodes in reciprocal space are referred to three orthogonal x, y, z axes, coinciding with the three twofold axes of the icosahedron. The x, y, z coordinates of a reciprocal-lattice vector, whose Miller indices are $n_1, n_2, n_3, n_4, n_5, n_6$, are given in this paper by

$$\mathbf{G}_{\parallel} = K \sum_{i=1}^6 n_i \mathbf{e}_{\parallel}^i, \quad (1)$$

where

$$K = 1/[2\pi a(1 + \tau^2)^{1/2}], \quad \tau = \frac{(1 + 5^{1/2})}{2}, \quad (2)$$

* In this work we label Bragg spots with the sixfold Miller indices notation due to Elser (1986).