No. 1A-4 $NaTaO_3$, Sodium tantalate
(M = 251.94)

1a Ferroelectricity in $NaTaO_3$ below 480 °C was reported by Matthias in 1949. 49Mat
No dielectric anomaly, however, was observed by Smolenskii et al. 57Smo

b

phase	IV	III	II	I	
state	(F)				
crystal system	orthorhombic	orthorhombic	tetragonal	cubic	57Kay
space group	Pcmn – D_{2h}^{5} [a])	Bmmb – D_{2h}^{17} [a])	P4/mbm – D_{4h}^{5} [a])		[a])80Aht
Θ [°C]	480	550	630		62Ism

3a Unit cell parameters: 80Aht
phase IV: a_o = 5.4842(2) Å, b_o = 7.7952(2) Å, c_o = 5.5213(2) Å at RT,
phase III: a_p = 7.8453(5) Å, b_p = 7.8541(8) Å, c_p = 7.8633(5) Å at 803 K,
phase II: $a_t = b_t$ = 5.5552(3) Å, c_t = 3.9338(4) Å at 893 K.

The subscripts o, p, and t mean orthorhombic, pseudocubic and tetragonal, respectively. These parameters are related to the primitive cubic perovskite unit cell parameter a as follows:

$a_o \approx \sqrt{2}a$, $b_o \approx 2a$, $c_o \approx \sqrt{2}a$; $a_p \approx 2a$, $b_p \approx 2a$, $c_p \approx 2a$; $a_t = b_t \approx \sqrt{2}a$ and $c_t \approx a$.

b Crystal structure: Tables 1A-4-001, 1A-4-002, 1A-4-003; Figs. 1A-4-001, 1A-4-002, 1A-4-003, 1A-4-004.

4 Thermal expansion: Table 1A-4-004; Fig. 1A-4-005.

11 Electrical conductivity: Fig. 1A-4-006.

13c Mössbauer effect: Table 1A-4-005; Fig. 1A-4-007.

16 Twin structure: see 90Uli

Table 1A-4-001. $NaTaO_3$. Structure of phase II [80Aht]. Fractional coordinates of atoms. T = 893 K. $B_{eq} = (B_{11} + B_{22} + B_{33})/3$ [75Wil]. R_{nucl}, R_{prof} and $R_{expected}$ are discrepancy factors in the neutron powder diffraction structure analysis.

		x	y	z	B [Å^2]
Isotropic temperature factor refinement					
Ta	2(a)	0	0	0	0.84(3)
Na	2(c)	0	½	½	3.91(7)
O(1)	2(b)	0	0	½	2.61(18)
O(2)	4(g)	¼+0.0231(5)	¼–0.0231	0	2.70(8)
		R_{nucl} = 13.48 %, R_{prof} = 21.39 %, $R_{expected}$ = 5.92 %			
					B_{eq} [Å^2]
Anisotropic temperature factor refinement					
Ta					0.98(13)
Na					3.92(31)
O(1)					3.21(23)
O(2)			u_2=0.0205(4)		2.86(13)
		$a_T = b_T$ = 5.5552(3) Å, c_T = 3.9338(4) Å			
		R_{nucl} = 6.45 %, R_{prof} = 14.61 %, $R_{expected}$ = 5.88 %			

Table 1A-4-002. $NaTaO_3$. Structure of phase III [80Aht]. Fractional coordinates of atoms. T = 803 K. $B_{eq} = (B_{11} + B_{22} + B_{33})/3$ [75Wil]. $R_{nucl,}$ R_{prof} and $R_{expected}$ are discrepancy factors in the neutron powder diffraction structure analysis.

		x	y	z	B [Å^2]
Isotropic temperature factor refinement					
Ta	8(d)	¼	0	¼	0.78(3)
Na(1)	4(c)	0	1	-0.021(5)	4 98(62)
Na(2)	4(c)	0	¼	½+0.008(5)	2.44(71)
O(1)	8(e)	¼+0.0185(12)	0	0	1.89(11)
O(2)	8(r)	0	0.0204(11)	¼–0.0318(12)	1.73(13)
O(3)	8(g)	¼–0.0241(11)	¼	¼–0.0023(13)	2.40(11)
		R_{nucl} = 11.97 %, R_{prof} = 17.07 %, $R_{expected}$ = 5.95 %			
					B_{eq} [Å^2]
Anisotropic temperature factor refinement					
Ta					0.097(17)
Na(1)		w_{A1} = –0.009(4)			3.65(76)
Na(2)		w_{A2} = –0.025(2)			2.65(72)
O(1)		u_1 = 0.0238(13)			2.07(29)
O(2)		u_2 = 0.0131(17),	w_2 = –0.0242(14)		3.00(36)
O(3)		u_3 = 0.0256(11),	w_3 = 0.0016(10)		2.28(32)
		a_p = 7.8453(5) Å, b_p = 7.8541 (8) Å, c_p = 7.8633(5) Å			
		R_{nucl} = 6.23 %, R_{prof} = 12.93 %, $R_{expected}$ = 5.93 %			

Table 1A-4-003. $NaTaO_3$. Structure of phase IV [80Aht]. Fractional coordinates of atoms. T = RT. $B_{eq} = (B_{11} + B_{22} + B_{33})/3$ [75Wil]. R_{nucl}, R_{prof} and $R_{expected}$ are discrepancy factors in the neutron powder diffraction structure analysis.

		x	y	z	B [Å^2]
Isotropic temperature factor refinement					
Ta	4(b)		0	0	0.384(14)
Na	4(c)	–0.0031(12)	¼	–0.01117(9)	1.507(34)
O(1)	4(c)	½–0.0599(4)	¼	0.0074(5)	0.842(29)
O(2)	8(d)	¼+0.0357(3)	–0.0295(2)	¼+0.0345(3)	0.897(18)
R_{nucl} = 6.56 %, R_{prof} = 12.41 %, $R_{expected}$ = 4.86 %					
					B_{eq} [Å^2]
Anisotropic temperature factor refinement					
Ta					0.53(13)
Na	u = –0.0047(11),	w = –0.0158(8)			1.42(32)
O(1)	u_1 = –0.0619(5),	w_1 = 0.0092(5)			0.82(18)
O(2)	u_2 = –0.0351(3),	υ_2 = 0.0295(2),	w_2 = 0.0340(3)		0.91(7)
a_o = 5.4842(2) Å, b_o = 7.7952(2) Å, c_o = 5.5213(2) Å					
R_{nucl} = 4.63 %, R_{prof} = 10.64 %, $R_{expected}$ = 4.85 %					

Table 1A-4-004. $NaTaO_3$. Temperature dependence of the pseudo-cell parameters [62Ism].

T [°C]	23	100	200	300	400	450	480	500
$a' = c'$ [Å]	3.889(5)	3.893(6)	3.899(5)	3.907	3.912(8)	3.916	3.918	3.920
b' [Å]	3.885(5)	3.890(5)	3.896(5)	3.903(8)	3.910(2)	3.913(6)	3.915(8)	3.918
β–90°	22'0"	16'00"	9'00"	6'0"	4'00"	3'30"	2'00"	≈2'00"
a'/b'	1.0010	1.0009	1.0009	1.0008	1.0006	1.0006	1.0005	1.0005
V [Å^3]	58.8(0)	59.0(0)	59.2(5)	59.5(5)	59.8(5)	60.0(0)	60.1(0)	60.2(0)

T [°C]	550	580	600
$a' = c'$ [Å]	3.923	3.925(2)	3.927
b' [Å]	3.923	≈3.925(2)	≈3.927
β–90°	1'30"	0'00"	0'00"
a'/b'	1.000	1.000	1.000
V [Å^3]	60.3(5)	60.4(5)	60.5(5)

T [°C]	630	660	680
$b = a = c$ [Å]	3.929	3.931	3.932(5)
V [Å^3]	60.6(5)	60.7(5)	60.8(0)

Table 1A-4-005. $NaTaO_3$. Mössbauer parameters [78Wor]. δ: isomer shift, e^2qQ: quadrupole splitting, η: asymmetry parameter.

T [K]	δ [$\cdot 10^{-3}$ m s^{-1}]	e^2qQ (7/2) [$\cdot 10^{-3}$ m s^{-1}]	η
77	–16.05(10)	+22.7(3)	0.55(10)
295	–15.45(10)	+18.2(2)	0.50(10)
418	–14.88(10)	+13.1(6)	0.50 fixed
565	–14.20(15)	+7.8(8)	0.50 fixed
700	–13.6(2)	5	0.50 fixed

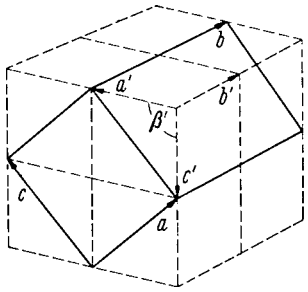

Fig. 1A-4-001. $NaTaO_3$. Othorhombic unit cell (full line) and primitive pseudo-monoclinic cells (broken line) in phase IV [57Kay]. a', b', c', β': lattice parameters of the pseudo-monoclinic cell.

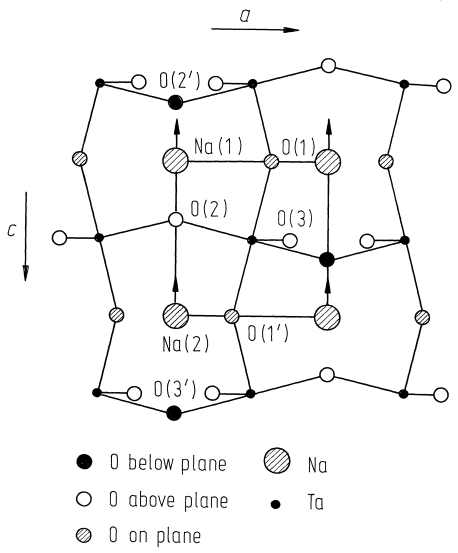

Fig. 1A-4-002. $NaTaO_3$. Structure of phase III [80Aht]. Projection of one of the atomic layers on the (010) plane. Short arrows indicate displacements of Na atoms. The displacements are antiparallel in successive layers perpendicular to [010].

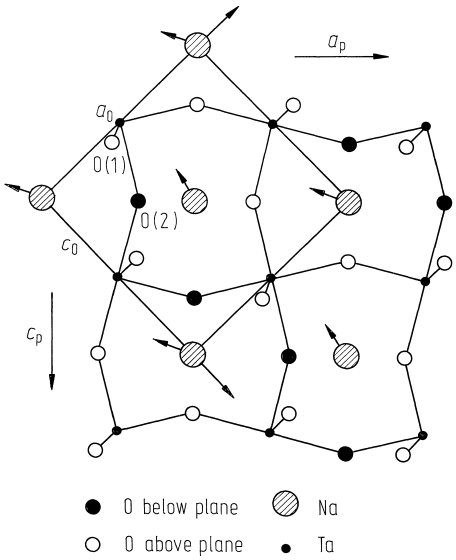

Fig. 1A-4-003. $NaTaO_3$. Structure of phase IV [80Aht]. Projection of one of the atomic layers on the (010) plane. a_o, c_o: orthorhombic unit cell vectors, a_p, c_p: pseudocubic unit cell vectors. Short arrows indicate displacements of Na atoms. The displacements are antiparallel in successive layers perpendicular to [010].

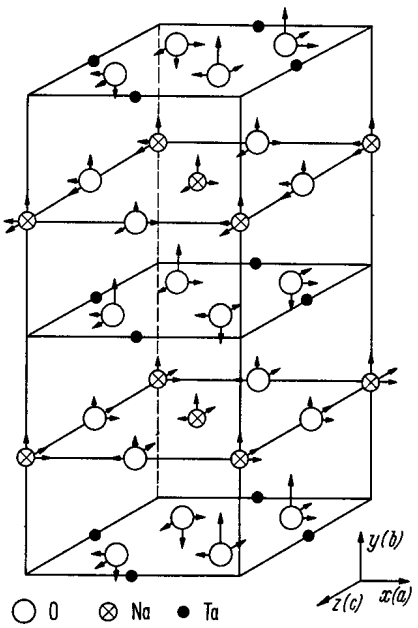

Fig. 1A-4-004. $NaTaO_3$. A sketch of the structure [57Kay]. The displacements of the ions from the cubic perovskite structure are indicated by arrows (exaggerated).

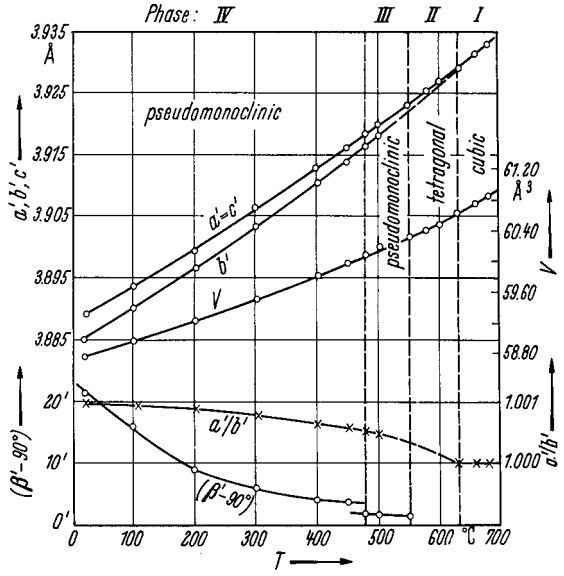

Fig. 1A-4-005. $NaTaO_3$. Lattice parameters vs. *T* [62Ism]. *a*', *b*', *c*', β': lattice parameters of the pseudomonoclinic cell.

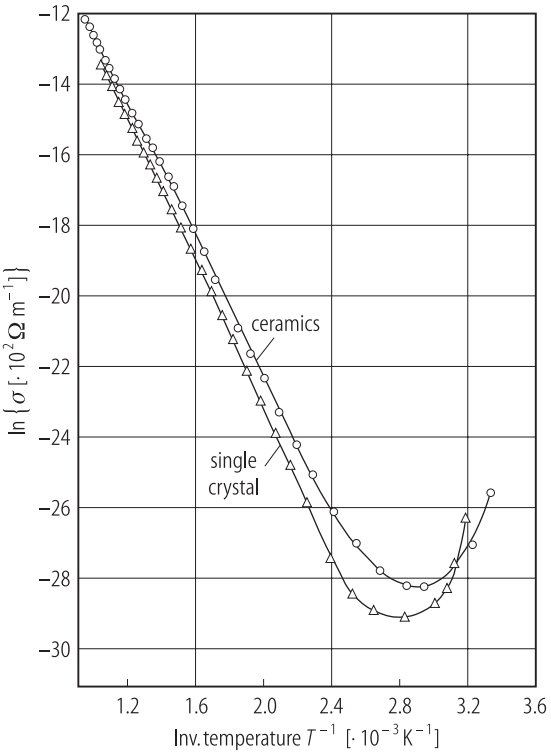

Fig. 1A-4-006. $NaTaO_3$. Electrical conductivity vs. $1/T$ [89Ale].

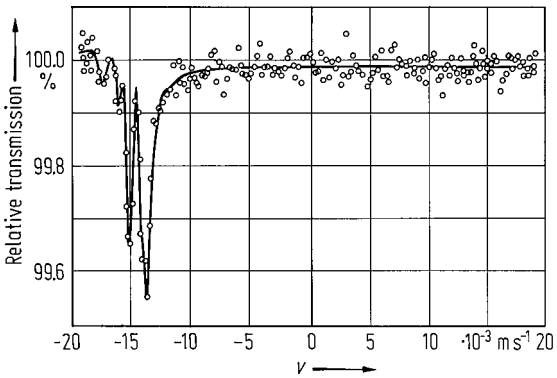

Fig. 1A-4-007. $NaTaO_3$. Mössbauer spectrum at 295 K [78Wor]. υ : source (^{181}W(W)) velocity. The solid line represents the fit of a quadrupole interaction with η = 0.45.

References

49Mat Matthias, B.T.: Phys. Rev. **75** (1949) 1771.

57Kay Kay, H.F., Miles, J.L.: Acta Crystallogr. **10** (1957) 213.

57Smo Smolenskii, G.A., Isupov, V.A., Arganovskaya, A.I., Sholokhovich, E.D.: Zh. Tekh. Fiz. **27** (1957) 2528; Sov. Phys. Tech. Phys. (English Transl.) **2** (1957) 2351.

62Ism Ismailzade, I.G.: Kristallografiya **7** (1962) 718; Sov. Phys. Crystallogr. (English Transl.) **7** (1963) 584.

75Wil Willis, B.T.M, Pryor, A.W.: Thermal Vibration in Crystallography, Cambrige University Press, 1975.

78Wor Wortmann, U., Trollmann, U., Heidemann, A., Kalvius, U.M.: Hyperfine Interact. **4** (1978) 610.

80Aht Ahtee, M., Darlington, C.N.W.: Acta Crystallogr., Sect. B **36** (1980) 1007.

89Ale Aleksandrowicz, A., Wojcik, K.: Ferroelectrics **99** (1989) 105 .

90Uli Ulinzheyev, A.V., Fesenko, E.G., Smotrakov, V.G.: Ferroelectrics **111** (1990) 261.