

No. 1A-10 BaTiO₃, Barium titanate $(M = 233.15)$

At about 1460 °C in air, cubic BaTiO₃ performs a transition to hexagonal phase. The reverse transition from the hexagonal to the cubic phase is very sluggish and the hexagonal form can be quenched into a practically stable state by relatively rapid cooling, especially in reducing atmosphere. Accordingly, there are two prototype structures of BaTiO₃ at room temperature: so-called cubic BaTiO₃ and hexagonal BaTiO₃. In this section, their data are presented separately as (i) cubic BaTiO₃ and (ii) hexagonal BaTiO₃.

(i) Cubic BaTiO₃

1a	The anomalous dielectric properties of BaTiO ₃ were discovered on ceramic specimens independently by Wainer and Solomon in 1942, by Ogawa in 1944 and by Wul in 1945. The ferroelectric activity of BaTiO ₃ was reported independently by von Hippel and co-workers in 1944 and by Wul in 1946. The structural change associated with the cubic-tetragonal phase transition was observed, by means of X-rays, by Megaw in-dependently of the above dielectric studies.					42Wai, 44Oga, 45Wul, 44von, 46Wul1, 45Meg
b	phase	IV ^{a)}	III ^{a)}	II ^{b)}	I ^{b)}	^{a)} 49Kay, 49Rho
	state	F ^{a)}	F ^{a)}	F ^{b)}	P ^{b)}	
	crystal system	rhombo-hedral ^{a)}	ortho-rhombic ^{a)}	tetragonal ^{b)}	cubic ^{b)}	hexagona ^{b)} 45Meg l ^{d)} ^{**)} ^{c)} 46von,
	space group	R3m – C _{3v} ⁵ ^{a)}	Amm2 – C _{2v} ¹⁴ ^{a)}	P4mm – C _{4v} ¹ ^{b)}	Pm3m – O _h ¹ ^{b)}	P6 ₃ / mmc – D _{6h} ⁴ ^{d)} 46Wul2 ^{d)} 55Ras ^{e)} 95Sak
	Θ [°C]	–90 ^{a)}	5 ^{a)}	123 ^{e)} [*]	1460 ^{d)}	
[*]) In most papers published earlier, the Curie point was reported to be about 120 °C. It was, however, reported to be about 130 °C in Ti-rich BaTiO ₃ [95Sak], as was observed in BaTiO ₃ single crystal pulled from Ti-rich melt [65Joh1]. ^{**}) The hexagonal form can be produced by rapid cooling from about 1460 °C in air. The transition temperature lowers to 1330 °C in a hydrogen atmosphere [60Gla], [69Are]. <i>P_s</i> [001] in phase II (along [100] of phase I). <i>P_s</i> [001] in phase III (along [110] of phase I). <i>P_s</i> [001] in phase IV (along [111] of phase I). The directions of <i>P_s</i> are illustrated along with lattice distortions in Fig. 1A-10-001. <i>T_{melt}</i> = 1620 °C. Tetragonal form (phase II): $\rho = 6.02 \cdot 10^3 \text{ kg m}^{-3}$ (calculated from lattice constants): see Transparent, light brown, straw-yellow color.						
2a	Crystal growth:					
	1) flux method (flux KF ^{a)} or TiO ₂ -rich melt ^{b)}); see					^{a)} 54Rem ^{b)} 65Sas, 67Bra

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- 2) pulling method (top-seeded solution growth technique using excess TiO₂ as the solvent); see 71Bel,
88Sch1,
92Aji
- 3) floating zone method (containing 3 mol% SrTiO₃); see 72Tie
- 4) solid-state grain growth method; see 94Yam2
- Phase diagram of BaO–TiO₂ system: Fig. 1A-10-002, Fig. 1A-10-003.
Solubility of BaTiO₃ in KF: Table 1A-10-001.
- Thin film growth:
- 1) vacuum evaporation; see 80Toc,
80Tom,
81Sev,
83Toc,
85Iij,
90Iij
- 2) sol-gel method; see 81Yan,
90Yok,
93Kuw,
93Hay
- 3) screen printing or electrophoresis and annealing; see 79Sur,
80Sur,
80Yam,
80Lop
- 4) sputtering method; see 79Pan,
80Pan,
81Dud1,
81Dud2,
81Ols,
79McC,
79Sur,
82Dha,
83Dha,
81Nag,
91Kle,
91Kaw
- 5) pulsed-laser deposition or laser ablation; see 89Dav,
91Nor,
92Roy,
93Kor,
93Nas,
94Wat
- 6) chemical vapor deposition; see 92Che,
91Nak,
91Kwa,
92Van,
93Kim,
94Kim,
95Kaw
- 7) hydrothermal method; see 90Ish,
91Kaj
- 8) molecular beam epitaxy; see 91McK

b Crystal forms: for butterfly type, Fig. 1A-10-004; for chunky type, Fig. 1A-10-005.	
3a Unit cell parameters:	
phase I: $a = 3.996 \text{ \AA}$ at 120°C .	47Miy,
phase II: $a = 3.9920 \text{ \AA}$, $c = 4.0361 \text{ \AA}$ at 20°C .	51Rho,
phase III: $a = 3.990 \text{ \AA}$, $b = 5.669 \text{ \AA}$, $c = 5.682 \text{ \AA}$ at -10°C .	57Shi,
phase IV: $a = 4.001 \text{ \AA}$, $\alpha = 89^\circ 51'$ at -168°C .	57Jon
b Crystal structure:	
phase I: $Z = 1^a$), Table 1A-10-002.	^a) 46Meg
phase II: $Z = 1^a$), Tables 1A-10-003, 1A-10-004, 1A-10-005; X-ray profile analysis.	80Tan, 78Gla
phase III: $Z = 2^b$), Table 1A-10-006; Fig. 1A-10-006, Fig. 1A-10-007.	^b) 57Shi
phase IV: $Z = 1^c$), Tables 1A-10-007, 1A-10-008, 1A-10-009.	^c) 74Hew
4a Thermal expansion: Figs. 1A-10-008, 1A-10-009, 1A-10-010; Table 1A-10-010. Lattice distortion due to p : Fig. 1A-10-011, Fig. 1A-10-012. Lattice distortion due to E : Fig. 1A-10-013. Lattice distortion in regard to particle size: Fig. 1A-10-014. Lattice constant in $\text{BaTiO}_{3-x}\text{F}_x$ ($0 < x < 0.1$); see Lattice constant in La doped ceramics (0 to 5 at%); see	90End 89Kle
5a Bulk crystal:	
Dielectric constant vs. T : Figs. 1A-10-015...1A-10-019. $C = 1.5(1) \cdot 10^5 \text{ K}$, $\Theta_p = 115^\circ\text{C}$.	65Joh1
Dielectric dispersion:	
1) $10^{-3} \dots 10^3 \text{ Hz}$; the dispersion was attributed to the surface layer with the thickness smaller than 10^{-2} cm .	78Dud1
2) $10^2 \dots 10^{10} \text{ Hz}$; Figs. 1A-10-020...1A-10-023; see also:	94Laa
3) far infrared to visible region; Figs. 1A-10-024...1A-10-028.	
4) ultraviolet region; Fig. 1A-10-029.	
Effect of hydrostatic pressures p on κ : Figs. 1A-10-030...1A-10-033.	
Phase diagram in regard to p : Figs. 1A-10-034...1A-10-037.	
Phase diagram in regard to two-dimensional pressures: Fig. 1A-10-038.	
Phase diagram in regard to E_{bias} : Fig. 1A-10-039.	
p - T - E_{bias} phase diagram; see	85Neu
Effect of additives: Fig. 1A-10-040.	
Ceramics:	
Dielectric constant vs. T : Figs. 1A-10-041...1A-10-046.	
$C = 10.48 \cdot 10^4 \text{ K}$ in the wide T range of $\Theta_t < T < 400^\circ\text{C}$.	89Flo
κ' and $\tan \delta$ of ceramics prepared from titanate oxides (anatase and rutile); see	91Fes, 91Fer
Dielectric dispersion: Fig. 1A-10-047, Fig. 1A-10-048.	
Size effects (density, grain size, thickness): Figs. 1A-10-049...1A-10-054; see also	76Kin, 85Ari
Aging effect of ac electric field on κ' and $\tan \delta$:	
Fig. 1A-10-055, Fig. 1A-10-056; see also	92WuK1
Effects of additives: Table 1A-10-011;	80Taw
Al;	87Aru

	Mn; Fig. 1A-10-057, see also Co; Zr; Ce; La; BaTiO ₃ –Ni composite ceramics; BaTiO ₃ –LiFe ₅ O ₈ composite ceramics;	78Per1 90Arm, 78Mol 83Iss 91Pan1 92Emo 91Sar
	Thin film: Dielectric constant vs. T : Figs. 1A-10-058...1A-10-061. Dielectric dispersion: Fig. 1A-10-062.	
b	Nonlinear dielectric properties: Figs. 1A-10-063...1A-10-065; see also Effect of E_{bias} on κ : Fig. 1A-10-066.	85Neu
c	Spontaneous polarization: Figs. 1A-10-067...1A-10-069. Coercive field: Fig. 1A-10-070. Grain size effect on spontaneous polarization and coercive field in ceramics: Figs. 1A-10-071...1A-10-074. Thin film: film thickness 220 nm, substrate Si single crystal, deposition temperature 650 °C; $P_r = 15.9 \cdot 10^{-2} \text{ Cm}^{-2}$, $E_c = 10.2 \cdot 10^5 \text{ Vm}^{-1}$; see	93Des
d	Electrocaloric effect: Fig. 1A-10-075. Pyroelectricity: Fig. 1A-10-076, Fig. 1A-10-077.	
6a	Heat capacity: Figs. 1A-10-078...1A-10-080; see also Transition heat, transition entropy: Table 1A-10-012.	73Str
b	Thermal conductivity: Figs. 1A-10-081...1A-10-083; see also	71Man
7a	Piezoelectricity: Tables 1A-10-013...1A-10-016; Fig. 1A-10-084, Fig. 1A-10-085; see also	59Hui, 50Cas
b	Electrostriction: Fig. 1A-10-086, Fig. 1A-10-087.	
8a	Elastic compliances and stiffnesses: Tables 1A-10-015...1A-10-017; see also Table 1A-10-014; for single crystal: see Figs. 1A-10-088...1A-10-093; for ceramics: see Figs. 1A-10-094...1A-10-096.	
b	Nonlinear elastic properties: Fig. 1A-10-097, Fig. 1A-10-098.	
9a	Refractive indices: Tables 1A-10-018...1A-10-021; Figs. 1A-10-099...1A-10-103. Birefringence: Tables 1A-10-018, 1A-10-021; Figs. 1A-10-104...1A-10-107. Reflection and absorption: 1) far-infrared region: Figs. 1A-10-108...1A-10-111. 2) infrared region: Fig. 1A-10-112. IR absorption due to OH bands: Fig. 1A-10-113. IR absorption due of Nb doped single crystals. IR absorption due of La or Yb doped ceramics. IR power spectra with different particle shapes.	81Mor 90Nas 89Dia

	3) visible region: Fig. 1A-10-114, Fig. 1A-10-115. with additives: Figs. 1A-10-116...1A-10-120.	
	4) ultraviolet region: Figs. 1A-10-121...1A-10-126; see also Table 1A-10-022. Effects of pressure on the absorption edge: see	59Suc
b	Effects of E_{bias} on the absorption edge: Figs. 1A-10-127...1A-10-129. Linear electrooptic effect: Fig. 1A-10-130, Fig. 1A-10-131; Tables 1A-10-023...1A-10-025. Electrooptic constants for different λ : see	67Zhe
	$r_{\lambda i}$ for different values of ac electric fields: see	89Jul
	$r_{\lambda i}$ of reduced and oxidized crystals: see	90Jul
	r_{42} in the temperature range of 18.5...19.5 °C : see	92Abd
	Quadratic electrooptic effect: Figs. 1A-10-132...1A-10-135.	
c	Piezoelectric effect: Fig. 1A-10-136; Table 1A-10-025.	
d	Faraday rotation: Fig. 1A-10-137; Table 1A-10-026.	
e	Optical SHG susceptibilities: Fig. 1A-10-138, Fig. 1A-10-139; $\left d_{15} / d_{36}^{\text{KDP}} \right = 35(3)$, $d_{31} / \left d_{36}^{\text{KDP}} \right = -37(3)$, $d_{33} / \left d_{36}^{\text{KDP}} \right = -14(1)$ at RT, for $\lambda = 1.0582 \mu\text{m}$; see	63Mil
	For absolute signs, see	70Mil
	Two photon absorption coefficient: Fig. 1A-10-140; see also	90Bog
10a	Raman scattering: Figs. 1A-10-141...1A-10-147; Table 1A-10-027; for scattering of the central-peak: Fig. 1A-10-148; for reduced and doped ceramics: Figs. 1A-10-149...1A-10-151; for powder with size of 10 nm...1 μm : see	94Sch
	Hyper-Raman scattering: Fig. 1A-10-152. Polariton: Figs. 1A-10-153...1A-10-156. Time-resolved spectroscopy of the soft modes: Fig. 1A-10-157.	
b	Brillouin scattering: Fig. 1A-10-158. Rayleigh scattering: Fig. 1A-10-159; see also	78Loo
11	Electrical conductivity σ of BaTiO_3 depends on various factors such as method of synthesis, crystal state (single or polycrystal), ferroelectric domain configuration, material used as electrode, aging, etc.: information concerning such factors may be obtained; see	69Gur
	Conductivity of as-grown crystals and ceramics: Figs. 1A-10-160...1A-10-164. Conductivity associated with doping or reduction: Figs. 1A-10-165...1A-10-174. There appears a temperature range near the Curie point where $d\rho/dT > 0$ (ρ : resistivity) in doped or reduced ceramics. Recent articles on the semiconductor ceramics with positive temperature coefficient of ρ : see	88AIA1, 89Che, 94Gil1, 88AIA2, 91Pan2, 88AIA3, 89Sin
	σ vs. oxygen pressure p_{O_2} : Fig. 1A-10-175, Fig. 1A-10-176; see also	76Dan1, 76Hen, 93Osa

	Effect of cation ratio Ba/Ti (0.99...1.01) on σ : see	89Rad
	Effect of hydrostatic pressure on σ : Fig. 1A-10-177; see also	69Wem
	Piezoresistivity: see	63Mat
	Relationship between σ and absorption coefficient: Fig. 1A-10-178.	
	Hall mobility: Fig. 1A-10-179, Fig. 1A-10-180; see also	76Ibr, 74Gru, 69Wem
	Drift mobility: see	79Boy
	Seebeck effect: Fig. 1A-10-181, Fig. 1A-10-182; see also	78Ihr
	Effective mass: $m^* = 6.5(2) \cdot m_0$ in n-type crystals; see also	67Ber 79Boy, 69Wem
	Breakdown field: Fig. 1A-10-183, Fig. 1A-10-184; see also	89Shi, 84Dak, 75Sch, 64Ued, 64Kaw
	Positron annihilation spectra: Fig. 1A-10-185.	
	X-ray and ultraviolet photoelectron spectra: Fig. 1A-10-186, Fig. 1A-10-187; Table 1A-10-028.	
	Photoconductivity and photoemission: Figs. 1A-10-188...1A-10-190; see also	90Mah
	Luminescence: Figs. 1A-10-191...1A-10-193; see also	86Kos
	Band structure: Fig. 1A-10-194; see also	67Bre, 91Cas, 92Coh, 94XuY
	Ba is essentially a fully Ba ²⁺ ion, while Ti 3d states hybridize with O 2p states: see	92Coh
12	Effect of intense magnetic field on Θ_f : Fig. 1A-10-195; the effect is very small; $\Delta\Theta_f \approx 0.2...0.3$ K at 200 kOe; see also	81Wag 84Ism, 82Fle
	Effect of intense magnetic field on κ : Fig. 1A-10-196.	
13a	NMR: Fig. 1A-10-197, Fig. 1A-10-198.	
b	ESR spin Hamiltonian parameters: Table 1A-10-029, Table 1A-10-030; Figs. 1A-10-199...1A-10-204. ESR linewidth vs. T : Fig. 1A-10-205, Fig. 1A-10-206. ESR study for light-sensitive centers: see	92Sch, 92Pos, 94Pos, 94War
	ESR study in semiconducting ceramics: see	85Kut
c	Mössbauer effect: Figs. 1A-10-207...1A-10-211; see also	80Wid, 85Her
14a	Bragg reflections due to structural modulation: Fig. 1A-10-212, Fig. 1A-10-213;	
b	Diffuse electron scattering: see	64Hon, 66Har

Diffuse X-ray scattering: Fig. 1A-10-214; see also 67Har1,
68Com1,
68Com2,
70Com,
71Com

Inelastic neutron scattering:
for cubic phase: Figs. 1A-10-215...1A-10-222;
for tetragonal phase: Figs. 1A-10-223...1A-10-225.

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- 15a Domain structure: Figs. 1A-10-226...1A-10-228.
Domains have been observed by various methods.
- 1) Polarized light: see 48Mat,
49For,
84Bor
 - 2) Etching method: Fig. 1A-10-229; see also 55Hoo
Etchant for revealing domain structure; hydrochloric acid or hydrofluoric acid; see 59Pea,
86HuY
 - 3) Powder pattern technique: see 59Pea
 - 4) Decoration technique: see 66Saw
 - 5) X-ray topography: see 64Nii,
65Cas,
81Kaw,
64Lam
 - 6) Transmission electron microscope: see 64Tan,
66Rem,
67Rem,
86HuY
 - 7) Scanning electron microscope: see 72LeB,
83Ari
 - 8) Photoemission microscope: see 70Mor,
70LeB
 - 9) Acoustic microscope: see 85Koj
 - 10) Electron-mirror microscope: see 70Som
 - 11) Nematic liquid crystal: see 93Bie1
 - 12) Interferometric study of 90° domains: see 61Bhi,
63Bhi
- Domain boundary has been studied by several methods.
- 1) Transmission electron microscope: see 76Mal,
92Tsa1,
92Shi
 - 2) Reflection electron microscope: see 92Tsa2
 - 3) Electron holographic study: see 94Zha2,
93Zha
- (111) twin boundary was studied by high-resolution transmission electron microscopy
and electron-energy-loss spectroscopy: see 94Rec
- Domain structure in crystals grown from high-temperature solution: see 94Par1,
94Par2
- Variation of domain structure with temperature change: see 85Beu,
93Bie1
- Formation of domain structure at P–F phase transition: see 78Sur,
86Gav,
84Bur,
86Bur

Influence of illumination on the domain structure: see	72Fri, 94Cud
Electro luminescence and light emission associated with domain switching: see	80Gon, 81Fle
Domain structure of ceramics was observed by etching method: Fig.1A-10-230; and by transmission electron microscope; see	89Kas
Domain structure of thin film: see	72Yak, 94Tsa
Domain structure of fine crystal and powder: see	93Hsi, 94Boc
b Domain wall motion was studied by following methods.	
1) Optical method: see	54Mer, 60Sav
2) Successive-etching method: see	63Sta, 64Sta
3) X-ray topography: see	79Tak
4) Transmission electron microscope: see	70Sha
The domain shapes in motion depend on the applied field and temperature: see	64Sta, 84Lee
The wall velocity is proportional to $\exp(-\delta/E)$ at relatively low field. δ is an activation field for domain wall motion: Figs. 1A-10-231...1A-10-237.	
Effect of elastic stress on domain structure: see	90Bor
Influence of polishing on the domain structure: see	88Beu
16 Surface:	
The first suggestion about the existence of surface layers of BaTiO ₃ crystal was made by Känzig ^{a)} on the basis of electron diffraction studies of very small particles of BaTiO ₃ ^{b)} .	^{a)} 55Kan ^{b)} 54Ani
Structure of surface layers have been studied by following diffraction methods.	
1) Electron diffraction in thin single crystals ^{c)} : the thickness of the layer was estimated to be very thin.	^{c)} 64Tan
2) LEED experiment ^{d)} : several superlattice structures were observed on the (100) surface in a wide range of temperature from RT up to 1000 °C.	^{d)} 71Abe1, 71Abe2
3) Electron mirror microscope ^{e)} : estimated thickness $\approx 0.7 \mu\text{m}$.	^{e)} 68Eng
The dependence of the following quantities on the thickness of the crystal has been observed as evidence of the existence of surface layers.	
1) Switching time: see	56Mer, 59Dro
2) Optical absorption coefficient: estimated thickness $\approx 6 \mu\text{m}$; see	60Cou
3) Dielectric dispersion: see	61Sch
4) Permittivity: estimated thickness $\approx 12 \mu\text{m}$; see	62Cou
Several anomalies due to existence of surface space charge layer have been observed under externally applied field.	
1) Electroluminescence (rf electric field): estimated thickness; $\approx 0.35 \mu\text{m}$; see	58Har
2) Electron emission: see	93Bie2
3) Birefringence: see	60Tri
4) Domain wall velocity: see	65Cal, 71Deg
5) Pyroelectricity: estimated thickness $\approx 0.1 \mu\text{m}$; see	56Chy2
6) Resistivity change: see	68Buc

7) X-ray diffraction: estimated thickness $\approx 1.5 \mu\text{m}$; see	72Mot, 78Dud2
8) Theoretical discussion about surface layers: see	59Jan, 59Dvo
 Anomalous mean square atomic displacement, thermal expansion and Grüneisen constant by LEED for (001) surface: see	 81Lub
Anomalous surface charge layer by double Laue pattern topography using synchrotron X-ray radiation: see	84Bor
 Radiation damage: Fig. 1A-10-238, Fig. 1A-10-239; see also	 66Hau, 57Wit
 Photorefractive effect:	
1) Decay rate: see	83Val, 84Duc
2) Effect of Fe doping: see	86God
3) Amplitude and phase of the photorefractive field: see	91Law
4) Intensity dependent absorption and photorefractive phenomena: see	88Bro, 87Mot, 90Bro, 90Tem, 91Tem
5) Intensity dependent photogalvanic effect: see	92Cud
6) Performance of 45° -cut crystal: see	89For, 92Zhu
7) Self-pumped phase-conjugation: see	85Gun, 87Eas, 88Gow, 94Yan

Table 1A-10-001. BaTiO₃. Solubility in KF solution [54Kar].

T [°C]	1000	1050	1100	1150	1200	1250	1300
BaTiO ₃ [mol %]	4	6	9	12.5	17	22.5	28.5

Table 1A-10-002. BaTiO₃. Fractional coordinates of atoms in the unit cell of phase I [52Meg].

	x	y	z
Ba	0	0	0
Ti	1/2	1/2	1/2
O	1/2	1/2	0
	1/2	0	1/2
	0	1/2	1/2

Table 1A-10-003. BaTiO₃. Fractional coordinates of atoms in the unit cell of phase II [70Har, 71Fra]. See also [78Gla].

	x	y	z	Δ_z^*	Δ_z^{**}	β_{33}^*	β_{33}^{**}	β_{11}^*	β_{11}^{**}	β_{22}^*	β_{22}^{**}
						[Å ²]					
Ba	0	0	0			0.32(7)	0.34(4)	0.51(6)	0.53(6)		
Ti	1/2	1/2	1/2+ Δ_z (Ti)	0.0135(4)	0.0135	0.32(2)	0.33(4)	0.30(2)	0.27(6)		
O(1)	1/2	1/2	Δ_z [O(1)]	-0.024(1)	-0.0250(4)	0.32	0.32(3)	0.57	0.57(6)		
O(2)	1/2	0	1/2+ Δ_z [O(2)]	-0.0150(9)	-0.0150(3)	0.32	0.33(3)	0.67	0.67(1)	0.56	0.56(1)
O'(2)	0	1/2	1/2+ Δ_z [O(2)]								

^{*}) X-ray diffraction data. ^{**}) Neutron diffraction data.

Table 1A-10-004. BaTiO₃. Interatomic distances in phase II [70Har].

Bond lengths	[Å]	Atomic shifts	[Å]
Ti–O(1)	2.1720	$\Delta_z(\text{Ti})$	0.0544
Ti–O(2)	2.0300	$\Delta_z[\text{O}(1)]$	0.1008
Ba–O(1)	2.8425	$\Delta_z[\text{O}(2)]$	0.0617
Ba–O(2)	2.7948		

Table 1A-10-005. BaTiO₃. Fractional coordinates of atoms in the unit cell of phase II [88Jia].

	x	y	z	$B [\text{\AA}^2]$
Ba	0.000	0.000	0.000	4.5(1)
Ti	0.500	0.500	0.515(5)	5.2(3)
O(1)	0.521(6)	0.521(6)	−0.031(3)	4.1(3)
O(2)	0.000	0.500	0.481(3)	4.4(1)

Table 1A-10-006. BaTiO₃. Fractional coordinates of atoms in the unit cell of phase III [57Shi].

	x	y	z
Ba	0	0	0
	0	1/2	1/2
Ti	1/2	0	1/2+ Δz_{Ti}
	1/2	1/2	Δz_{Ti}
O(1)	0	0	1/2+ $\Delta z_{\text{O}(1)}$
	0	1/2	$\Delta z_{\text{O}(1)}$
	1/2	1/4+ $\Delta y_{\text{O}(2)}$	1/4+ $\Delta z_{\text{O}(2)}$
O(2)	1/2	3/4+ $\Delta y_{\text{O}(2)}$	3/4+ $\Delta z_{\text{O}(2)}$
	1/2	3/4- $\Delta y_{\text{O}(2)}$	1/4+ $\Delta z_{\text{O}(2)}$
	1/2	1/4- $\Delta y_{\text{O}(2)}$	3/4+ $\Delta z_{\text{O}(2)}$

$\Delta z_{\text{Ti}} = +0.010$; $\Delta z_{\text{O}(1)} = -0.010$;
 $\Delta z_{\text{O}(2)} = -0.013$; $\Delta y_{\text{O}(2)} = +0.003$.

Table 1A-10-007. BaTiO₃. Fractional coordinates of atoms in the unit cell of phase IV [74Hew]. Neutron powder profile analysis; lattice parameters a , b , c , α , β , γ and scattering lengths b_{Ba} , b_{Ti} , b_{O} were also refined in the analysis.

	x	y	z
Ba	$\Delta_z(\text{Ba})$	$\Delta_z(\text{Ba})$	$\Delta_z(\text{Ba})$
Ti	$1/2 + \Delta_z(\text{Ti})$	$1/2 + \Delta_z(\text{Ti})$	$1/2 + \Delta_z(\text{Ti})$
O(1)	$1/2 + \Delta_z(\text{O})$	$1/2 + \Delta_x(\text{O})$	$\Delta_z(\text{O})$
O(2)	$1/2 + \Delta_z(\text{O})$	$\Delta_z(\text{O})$	$1/2 + \Delta_x(\text{O})$
O(3)	$\Delta_z(\text{O})$	$1/2 + \Delta_x(\text{O})$	$1/2 + \Delta_x(\text{O})$
<hr/>			
	$\Delta_z(\text{Ba}) = 0.013(3)$	$a = b = c = 4.001 \text{ \AA}$	
	$\Delta_z(\text{Ti}) = 0$	$\alpha = \beta = \gamma = 89.868(4)^\circ$	
	$\Delta_x(\text{O}) = 0.024(2)$	$b_{\text{Ba}} = 0.517(7) \cdot 10^{-12} \text{ cm}$	
	$\Delta_z(\text{O}) = 0.031(2)$	$b_{\text{Ti}} = 0.347(6) \cdot 10^{-12} \text{ cm}$	
	$B(\text{Ba}) = 0.26(8) \text{ \AA}^2$	$b_{\text{O}} = 0.58 \cdot 10^{-12} \text{ cm}$	
	$B(\text{Ti}) = 0.10(15) \text{ \AA}^2$		
	$B(\text{O}) = 0.24(3) \text{ \AA}^2$		

Table 1A-10-008. BaTiO₃. Atomic displacement in three phases [74Hew]. $\Delta(M)$:displacement of M atom relative to the fixed center of mass, where M stands for Ba, Ti or O. \parallel , \perp : parallel and perpendicular to the ferroelectric axis [hkl].

	tetr [001] 20 °C [70Har]	orth [001] −10 °C [57Shi]	rh [111] 77.4 K [74Hew]	
$\Delta_{\parallel}(\text{Ba})$	0.004	0.002	0.001(21)	[Å]
$\Delta_{\parallel}(\text{Ti})$	0.058(2)	0.059	0.091	[Å]
$\Delta_{\parallel}(\text{O}_I)$	−0.093(4)	−0.055	−0.091(14)	[Å]
$\Delta_{\parallel}(\text{O}_{II})$	−0.057(4)	−0.072	−0.091	[Å]
$\Delta_{\parallel}(\text{O}_{III})$	−0.057	−0.072	−0.091	[Å]
$\Delta_{\perp}(\text{O}_I)$	0	0.017	0.023	[Å]

Table 1A-10-009. BaTiO₃. Fractional coordinates of atoms in the unit cell of phase IV [81Sch]. $a_{\text{rh}} = 4.004(3) \text{ \AA}$, $\alpha_{\text{rh}} = 89.87^\circ$, not refined. $\beta_{ij} [\text{\AA}^2]$: defined by Eq.(c) of Introduction.

Ba	0	0	0
$\beta_{11}(\text{Ba})$	0.0025(2)		$\rightarrow B = 0.162(12) \text{ \AA}^2$
$\beta_{12}(\text{Ba})$	0.0004(2)		
Ti	$1/2 - x_{\text{Ti}}$	$1/2 - x_{\text{Ti}}$	$1/2 - x_{\text{Ti}}$
x_{Ti}	0.0111(3)		
$\beta_{11}(\text{Ti})$	0.0017(2)		
$\beta_{12}(\text{Ti})$	0.0006(2)		$\rightarrow B = 0.112(12) \text{ \AA}^2$
O	$1/2 + x_{\text{O}}$	$1/2 + x_{\text{O}}$	z_{O}
x_{O}	0.0110(2)		
z_{O}	0.0180(2)		
$\beta_{11}(\text{O})$	0.0044(1)		
$\beta_{33}(\text{O})$	0.0036(1)		$\rightarrow B = 0.266(6) \text{ \AA}^2$
$\beta_{12}(\text{O})$	-0.0003(1)		
$\beta_{13}(\text{O})$	-0.0003(1)		

Table 1A-10-010. BaTiO₃. Unit cell parameters vs. T [81She].

Temperature interval [°C]	Crystal symmetry	Analytical expressions for thermal behaviour [Å]
–170 to –68.9	rhombohedral	$a = 4.00758 + 0.1881 \cdot 10^{-4} T$
–98.5 to 8.2	monoclinic	$a = 4.01566 - 0.2569 \cdot 10^{-4} T$ $c = 3.99021 + 0.1069 \cdot 10^{-3} T$
–5.9 to 121.4	tetragonal	$a = 3.99153 + 0.6284 \cdot 10^{-4} T$ $- 0.3443 \cdot 10^{-7} T^2 + 0.3495 \cdot 10^{-8} T^3$ $c = 4.03641 - 0.8647 \cdot 10^{-4} T$ $+ 0.9716 \cdot 10^{-6} T^2 - 0.9753 \cdot 10^{-8} T^3$
118.6 to 220	cubic	$a = 4.00692 + 0.1537 \cdot 10^{-4} T$ $+ 0.8277 \cdot 10^{-7} T^2$

Table 1A-10-011. BaTiO₃ with additives. Parameters of the dielectric dispersion in the Cole-Cole formula, $\kappa = \kappa_{\infty} + \Delta\kappa / \{1 + (i f / f_r)\}^{1-\alpha}$ [92Kaz]. f_r : the relaxation frequency.

	BaTi _{1-x} Zr _x O ₃		BaTi _{1-x} Hf _x O ₃		Ba _{1-y} Sr _y TiO ₃		
	x = 0.1	x = 0.2	x = 0.1	x = 0.2	y = 0.1	y = 0.2	y = 0.3
f_r [MHz]	300	90	350	80	450	730	450
$\Delta\kappa$	1280	11.10 ³	4800	26.10 ³	1100	1730	3360
κ_{∞}	480	2.10 ³	520	5.10 ³	610	100	960
α	0.19	0.28	0.27	0.05	0.01	0.05	0.01

	Ba _{1-y} Ca _y TiO ₃		Ba _{1-y} Pb _y TiO ₃			BaTi _{1-z} Li _z O _{3-3z} F _{3z}		
	y = 0.05	y = 0.1	y = 0.05	y = 0.1	y = 0.2	z = 0.025	z = 0.05	z = 0.01
f_r [MHz]	700	>10 ³	700	800	>10 ³	100	150	500
$\Delta\kappa$	1440	–	460	320	–	7900	3900	1630
κ_{∞}	520	–	490	270	–	900	1400	330
α	0.02	–	0.01	0.01	–	0.15	0.05	0.21

Table 1A-10-012. BaTiO₃. Transition heat and transition entropy.

Transition	ΔQ_m [J mol ⁻¹]	ΔS_m [J mol ⁻¹ K ⁻¹]	Ref.
IV→III	33.5(84)	0.17	52Shi
	59.8	0.29	52Vol
	50	0.25	52Tod
III→II	92(17)	0.318	52Shi
	64.8	0.226	52Vol
	67	0.242	52Tod
II→I	209(21)	0.523	52Shi
	196	0.50	52Vol
	196	0.50	48Bla

Table 1A-10-013. BaTiO₃ (single crystal and ceramics). Piezoelectric constants and electromechanical coupling factor [66Bec].

	d_{15}	d_{31}	d_{33}	g_{15}	g_{31}	g_{33}	k_{15}	k_{31}	k_{33}	k_p	T	Ref.
	[$\cdot 10^{-12} \text{ CN}^{-1}$]			[$\cdot 10^{-3} \text{ m}^2 \text{ C}^{-1}$]							[°C]	
single crystal		−57.7	132								20	50Cas
	392	−34.5	85.6	15.3	−23.1	57.6	0.570	0.315	0.560		25	58Ber
		−33.3										59Hui
		−103.3	316.6								RT	51Bon
ceramic	270	−79	191	18.8	−4.7	11.4	0.476	0.208	0.493	0.378	25	56Bec
	260	−78	190	20.2	−5.2	12.6	0.48	0.212	0.50	0.36	25	64Ber

	e_{15}	e_{31}	e_{33}	h_{15}	h_{31}	h_{33}	T	Ref.
	[Cm^{-2}]			[$\cdot 10^8 \text{ NC}^{-1}$]			[°C]	
ceramic	11.6	−4.4	18.6	10.3	−3.5	14.8	25	56Bec
	11.4	−4.35	17.5	11.5	−3.9	15.6	25	64Ber

Table 1A-10-014. BaTiO₃ (ceramics, plain and modified, commercial). Dielectric, piezoelectric, electromechanical and elastic constants (at 25 °C, except for Ca_{0.12}Pb_{0.08}Ba_{0.80}TiO₃) [66Bec].

Composition	κ_{33}^T	d_{15}	d_{31}	d_{33}	g_{15}	g_{31}	g_{33}	s_{11}^E	s_{12}^E	s_{66}
		[·10 ⁻¹² CN ⁻¹]			[·10 ⁻³ m ² C ⁻¹]			[·10 ⁻¹² m ² N ⁻¹]		
BaTiO ₃	1350		-56	130				8.47	-2.38	21.7
	...1700			...160						
Ca _{0.05} Ba _{0.95} TiO ₃ (ceramics B) ^{a)}	1200	242	-58	149	21.0	-5.5	14.1	8.6	-2.6	22.4
Pb _{0.05} Ba _{0.95} TiO ₃	1180		-53	129				9.09	-2.64	23.64
Ca _{0.06} Pb _{0.04} Ba _{0.90} TiO ₃	800		-40	115				8.06	-2.34	20.8
Ca _{0.08} Pb _{0.12} Ba _{0.80} TiO ₃	450		-20	60		-5.0	15.0	7.8	-2.3	20.2
Ca _{0.12} Pb _{0.08} Ba _{0.80} TiO ₃	600		-35	90		-7.3	18	13		

Composition	k_{15}	k_{31}	k_{33}	k_p	κ_{11}^T	κ_{11}^S	κ_{33}^S	e_{15}	e_{31}	e_{33}
	[Cm ⁻²]									
Ca _{0.05} Ba _{0.95} TiO ₃ (ceramics B) ^{a)}	0.48	0.194	0.48	0.33	1300	1000	910	10.9	-3.1	13.5
Ca _{0.08} Pb _{0.12} Ba _{0.80} TiO ₃	0.30	0.113	0.34	0.19			395			
Ca _{0.12} Pb _{0.08} Ba _{0.80} TiO ₃		0.12	0.30	0.22						

Composition	s_{11}^D	s_{33}^E	s_{33}^D	s_{12}^D	s_{13}^E	s_{13}^D	s_{44}^E	s_{44}^D	h_{15}	h_{31}	h_{33}
	[·10 ⁻¹² m ² N ⁻¹]								[·10 ⁸ NC ⁻¹]		
Ca _{0.05} Ba _{0.95} TiO ₃ (ceramics B) ^{a)}	8.3	9.1	7.0	-2.9	-2.7	-1.9	22.2	17.1	12.3	-3.8	16.7
Ca _{0.08} Pb _{0.12} Ba _{0.80} TiO ₃	7.7	8.1	7.15	-2.4							

Composition	c_{11}^E	c_{11}^D	c_{33}^E	c_{33}^D	c_{12}^E	c_{12}^D	c_{13}^E	c_{13}^D	c_{44}^E	c_{44}^D	c_{66}
	[·10 ⁹ Nm ⁻²]										
Ca _{0.05} Ba _{0.95} TiO ₃ (ceramics B) ^{a)}	158	159	150	177	69	70	67.5	62	45	58.5	45

^{a)} Trade Mark: Clevite Corporation, Cleveland, Ohio, USA.

Table 1A-10-015. BaTiO₃. Elastic and piezoelectric constants at 25 °C and 130 °C [86Sch].

T [°C]	25 ^{a)}	25	130	T [°C]	25 ^{a)}	25	130
κ_{33}	168.0	130.0	1783.00	$s_{13}^D [\cdot 10^{-12} \text{ m}^2 \text{ N}^{-1}]$	-3.26	-3.00	-0.14
κ_{11}	1970.00	4000.00	1960.00	s_{55}^D	12.40	7.36	9.59
$s_{11}^E [\cdot 10^{-12} \text{ m}^2 \text{ N}^{-1}]$	8.05	7.35	10.40	$d_{31} [\cdot 10^{-12} \text{ C N}^{-1}]$	-34.50	-33.40	-284.00
s_{33}^E	15.70	14.95	36.25	d_{33}	85.60	68.50	695.00
s_{12}^E	-2.35	-1.39	1.15	d_{15}	392.00	647.00	338.00
s_{13}^E	-5.24	-4.94	-11.62	$g_{31} [\cdot 10^{-2} \text{ V m N}^{-1}]$	-2.30	-3.00	-1.70
s_{55}^E	18.40	18.21	14.85	g_{33}	5.75	5.61	4.10
s_{66}	8.84	8.33	9.61	g_{15}	1.52	1.74	1.75
s_{11}^D	7.25	6.24	5.49	k_{31}	0.315	0.39	0.69
s_{33}^D	10.80	10.00	9.55	k_{33}	0.56	0.55	0.87
s_{12}^D	-3.15	-2.60	-2.40	k_{15}	0.57	0.75	0.60

^{a)} [58Ber].

Table 1A-10-016. BaTiO₃. Elastic and piezoelectric constants at 23 °C [94Zgo].

Parameter	Value	Parameter	Value	Parameter	Value
κ_{11}^T	4400(400)	c_{11}^D [$\cdot 10^9 \text{ Nm}^{-2}$]	223(10)	s_{11}^E [$\cdot 10^{-12} \text{ N}^{-1} \text{ m}^2$]	7.4(3)
κ_{33}^T	129(5)	c_{12}^D	109(5)	s_{33}^E	13.1(1.5)
κ_{11}^S	2200(200)	c_{13}^D	102(5)	s_{12}^E	−1.483
κ_{33}^S	56(3)	c_{33}^D	240(10)	s_{13}^E	−4.4(5)
d_{31} [$\cdot 10^{-12} \text{ CN}^{-1}$]	−33.4(20)	c_{55}^D	121(5)	s_{66}^E	7.6(8)
d_{33}	90(5)	c_{11}^E	222(10)	s_{55}^E	16.4(16)
d_{15}	564(40)	c_{12}^E	108(18)	s_{11}^D	6.4(3)
e_{31} [Cm^{-2}]	−0.7(6)	c_{13}^E	111(8)	s_{33}^D	5.6(10)
e_{33}	6.7(3)	c_{33}^E	151(7)	s_{12}^D	−2.3(4)
e_{15}	34.2(18)	c_{55}^E	61(3)	s_{13}^D	−1.7(3)
		c_{66}^E	134(6)	s_{55}^D	8.4(16)

Table 1A-10-017. BaTiO₃ (single crystal and ceramics). Elastic constants [66Bec].

	s_{11}^E	s_{11}^D	s_{33}^E	s_{33}^D	s_{12}^E	s_{12}	s_{13}^E	s_{13}^D	s_{44}^E	s_{44}^D	s_{66}	T	Ref.
	[$\cdot 10^{-12} \text{ m}^2 \text{ N}^{-1}$]											[°C]	
Single crystal	9.26											25	50Cas
	11.2											RT	51Bon
	8.05	7.25	15.7	10.8	-2.35	-3.15	-5.24	-3.26	18.4	12.4	8.84	25	58Ber
Ceramics	8.55	8.18	8.93	6.76	-2.61	-2.98	-2.85	-1.95	23.3	18.3	22.3	25	56Bec
	9.1	8.7	9.5	7.1	-2.7	-3.0	-2.9	-1.9	22.8	17.5	23.6	25	64Ber
	c_{11}^E	c_{11}^D	c_{33}^E	c_{33}^D	c_{12}^E	c_{12}^D	c_{13}^E	c_{13}^D	c_{44}^E	c_{44}^D	c_{66}	T	Ref.
	[$\cdot 10^9 \text{ Nm}^{-2}$]											[°C]	
Single crystal	275.1	282.6	164.9	178.1	179.0	186.5	151.6	141.6	54.34	80.64	113.1	25	66Bec, 58Ber
		206				140				126		RT	51Bon
Ceramics	166	168	162	189	76.6	78.2	77.5	71.0	42.9	54.6	44.8	25	56Bec
	150	150	146	171	66	68	66	57	44	57	43	25	64Ber
	165.6			180.7					42.48	53.02	45.65	25	55Hun

Table 1A-10-018. BaTiO₃. Refractive indices and birefringence [93Bus]. $T = 20\text{ }^{\circ}\text{C}$.

λ [nm]	n_e	n_o	$n_e - n_o$
488	2.447	2.520	-0.073
514	2.424	2.491	-0.067
532	2.410	2.474	-0.064
633	2.360	2.412	-0.052

Table 1A-10-019. BaTiO₃. Parameters of the Sellmeier equation [93Bus]. n_e , n_o : extraordinary and ordinary refractive indices. A , B , C : parameters in the equation of $n^2(\lambda) - 1 = A + \{B\lambda^2/(\lambda^2 - C)\}$.

T [°C]	n_e			n_o		
	A	B	$C [·10^{-14} \text{ m}^2]$	A	B	$C [10^{-14} \text{ m}^2]$
20	2.109	2.022	7.095	2.154	2.141	7.890
30	1.898	2.239	6.647	2.139	2.166	7.777
40	1.458	2.661	5.800	1.527	2.739	6.581
50	1.770	2.364	6.333	1.881	2.399	7.175
60	1.649	2.482	6.380	1.711	2.550	7.125
70	1.668	2.472	6.460	1.578	2.677	6.909
80	1.846	2.314	6.798	1.658	2.601	7.021

Table 1A-10-020. BaTiO₃. Thermooptic coefficient dn_e/dT for wavelength λ and temperature T [93Bus]. n_e : extraordinary refractive index.

T [°C]	dn_e/dT [$\cdot 10^{-5} \text{ K}^{-1}$]			
	$\lambda = 488 \text{ nm}$	$\lambda = 514 \text{ nm}$	$\lambda = 532 \text{ nm}$	$\lambda = 633 \text{ nm}$
20	26	25	23	18
40	28	25	23	19
60	37	34	33	30
80	56	51	49	41

Table 1A-10-021. BaTiO₃ (Fe doped). Refractive indices [86God]. $\lambda = 632.8$ nm. $T = \text{RT}$.

Iron concentration	"pure"	0.075%	0.125%
n_c	2.4060	2.4381	2.4100
n_a	2.4875	2.5277	2.4900
$ n_c - n_a $	0.0815	0.0896	0.0800

Table 1A-10-022. BaTiO₃, SrTiO₃, TiO₂. Energies of fundamental absorption edges [in eV] at RT [65Car].

	E ₀	A ₁	A ₂	A ₃	B ₁	B ₂	C ₁	C ₂	D	E	
SrTiO ₃	3.2	4.00	4.86	5.5	6.52	7.4	9.2	9.9	12.5	15.3	[eV]
BaTiO ₃	3.2	3.91	4.85		6.10	7.25	10.3	11.8	12.8	15	[eV]
TiO ₂ (<i>E</i> ⊥ <i>c</i>)		3.97	5.52		6.50	7.64	8.53	9.24	11	14.1	[eV]

Table 1A-10-023. BaTiO₃. Electrooptic constants [69Bec].

	r_{13}	r_{33}	r_{42}	$r_c = r_{33} - (n_d/n_c)^3 r_{13}$	T	λ	Ref.
	$[\cdot 10^{-12} \text{ mV}^{-1}]$				$[^{\circ}\text{C}]$	$[\text{nm}]$	
T			1640	108	25	546.1	65Joh2
S	8	28(5)		19		633	65Kam, 66Kam
S			820(100)	23(2)	25	546.1	65Joh3

Table 1A-10-024. BaTiO₃ (Fe doped). Electrooptic constant at constant strain [86God]. $\lambda = 632.8$ nm.

Iron concentration	pure	0.045%	0.075%	0.125%	0.250%
$r_{13} [\cdot 10^{-12} \text{ mV}^{-1}]$	11	24	96	60	126
$r_{33} [\cdot 10^{-12} \text{ mV}^{-1}]$	31	90	87	120	118
$r_{42} [\cdot 10^{-12} \text{ mV}^{-1}]$	1000	2900	7530	3700	5180

Table 1A-10-025. BaTiO₃. Piezooptic $p_{\lambda\mu}$ and electrooptic $r_{\lambda i}$ constants at 23 °C [94Zgo].
 $\lambda = 633$ nm. $n_a = 2.412$, $n_c = 2.360$.

p_{11}^E	p_{12}^E	p_{13}^E	p_{31}^E	p_{33}^E	p_{55}^E
0.50(4)	0.106(19)	0.200(14)	0.070(7)	0.77(4)	1.0(2)
$r_{13}^{\mathbf{S}}$	$r_{33}^{\mathbf{S}}$	$r_{42}^{\mathbf{S}}$	$r_{13}^{\mathbf{T}}$	$r_{33}^{\mathbf{T}}$	$r_{42}^{\mathbf{T}}$
[$\cdot 10^{-12} \text{ mV}^{-1}$]					
10.2(6)	40.6(25)	730(100)	8(2)	105(10)	1300(100)

Table 1A-10-026. BaTiO₃, SrTiO₃, KTaO₃, KTa_{0.35}Nb_{0.65}O₃ (KTN), TiO₂. Band gap energies $\hbar\omega_g$ [in eV] [67Bae]. F₁, F₂: different dispersion functions F₁(ω/ω_g). See Fig. 1A-10-137.

	SrTiO ₃		BaTiO ₃	KTaO ₃		KTN	TiO ₂	
	296 K	77 K	403 K	296 K	77 K	296 K	296 K	
Faraday rotation $\hbar\omega_g$ for F ₁	3.40	3.43	3.25	3.77	3.79	3.54	3.62	eV
Faraday rotation $\hbar\omega_g$ for F ₂	3.21	3.26	3.11	3.62	3.65	3.36	3.37	eV
Energy of reflectivity peak or shoulder	3.20	–	3.20	–	–	3.70	–	eV
Energy of electro- reflectance singularity	–	–	3.20	3.57 3.80	–	3.60	3.00 3.30	eV eV
$\hbar\omega_g$ from absorption data	3.40	–	–	3.75	–	–	–	eV
Energy at which absorption coefficient $\alpha \approx 10^4$ [cm ⁻¹]	3.37	–	3.26	3.79	–	3.45	3.18	eV

Table 1A-10-027. BaTiO₃. Optical-branch vibration mode assigned at 25 °C [68DiD]. The crystal was produced by the top-seeded solution technique.

Cubic re- presentation	Raman scattering data [$\cdot 10^2 \text{ m}^{-1}$]; accuracy $\pm 3 \cdot 10^2 \text{ m}^{-1}$							
	E(TO, <i>xy</i>)	E(TO, <i>z</i>)	E(LO, <i>xy</i>)	A ₁ (TO, <i>xy</i>)	A ₁ (LO, <i>z</i>)	E(TO+LO, <i>xy</i>)	E(TO+LO, <i>z</i>)	B ₁
F _{1u}	36	36	715	≈ 180	727	—	—	—
F _{1u}	180	180	180	80	178	—	—	—
F _{1u}	486	518	463	470	470	—	—	—
F _{2u}	—	—	—	—	—	305	305	305

Table 1A-10-028. BaTiO₃. X-ray photoelectron spectroscopic determination of core level binding energies to the O 1s level taken at 531.0 eV [78Per2].

Level	Binding energy [eV]	Level	Binding energy [eV]
O 1s	531.00	Ti 3p _{1/2} }	38.6(1)
Ti 2p _{1/2}	465.6(1)	Ti 3p _{3/2} }	
Ti 2p _{3/2}	459.8(1)	Ba 5s	30.5(1)
Ba 4d _{3/2}	92.5(1)	O 2s	23.0(1)
Ba 4d _{5/2}	89.8(1)	Ba 5p _{1/2}	16.7(1)
		Ba 5p _{3/2}	14.9(1)

Table 1A-10-029. BaTiO₃. Summary of ESR parameters for various paramagnetic centers in doped BaTiO₃.

*)	Site	<i>S</i>	H	<i>ν</i>	<i>T</i>	<i>g</i> -factor	FS: <i>D, E, a, F, b</i>			HFS:		Ref.
							[·10 ⁻² m ⁻¹]			<i>I</i>	<i>A, B</i> [·10 ⁻² m ⁻¹]	
Mn ²⁺	Ti ⁴⁺	5/2 (7)	9.3	9.3	78	2.0016(5)	<i>D</i> =56(5)			5/2	⁵⁵ <i>A</i> = ⁵⁵ <i>A</i> _⊥ ^{a)}	60Ism
					300	2.0023(5)	<i>D</i> =65(5)				⁵⁵ <i>A</i> =79.8(5)	
					440	2.0009(1)	<i>a</i> =14(5)				⁵⁵ <i>A</i> =78.6(5) ^{b)}	63Ode
	Ba ²⁺	5/2 (7)	9.3	9.3	RT	2.002(1)	<i>D</i> =+215(2) <i>E</i> =0				⁵⁵ <i>A</i> =79(5) ^{c)}	64Iku
					438	2.002(1)	<i>D</i> =0 <i>E</i> =0				⁵⁵ <i>A</i> =-77.4(6)	
Fe ³⁺	Ti ⁴⁺	5/2 (7)	5...7.5, 10,16.3 10	9.3	393,	2.003	<i>D</i> =0				⁵⁵ <i>A</i> = ⁵⁵ <i>A</i> _⊥	66Iku ¹⁾ 2)
					433		<i>a</i> =102(12)				⁵⁵ <i>A</i> =-79.3(4)	
					300	2.0036(2)	<i>D</i> =+929 <i>E</i> =0					59Hor, 62Rim
							<i>a</i> =+91(20)					63Sak ²⁾
					276	2.0036(2)	<i>D</i> =-530(10)					f)
							<i>a</i> =+105(20)					
					213	2.0036(2)	<i>D</i> =-640(10),					
							<i>E</i> =0.0(13)					
					77	2.0036(2)	<i>D</i> =0 <i>E</i> =0					
							<i>a</i> =+115(10)					
Co ²⁺	Ti ⁴⁺	1/2 (3)	9	9	4	4.347	<i>D</i> =-23(5)					64Sak ²⁾ 3)
						(isotropic)	<i>a</i> - <i>F</i> =+113(10)					
										7/3	⁵⁹ <i>A</i> = ⁵⁹ <i>A</i> _⊥ ⁵⁹ <i>A</i> =109	67Zda
Gd ³⁺	Ba ²⁺	7/2 (8)	12,18	12,18	300	1.995(3)	<i>b</i> ₂₀	<i>b</i> ₄₀	<i>b</i> ₆₀			62Rim
					425	1.995(3)	-	≈6	-			
	Ti ⁴⁺		10	10	RT	1.992	-	24.0(9)	-3.7(28)			64Tak
					436	1.992	-	23.3(4)	-1.8(4)			66Tak1
Pt ³⁺	Ti ⁴⁺	1/2 (3)	10	10	4	<i>g</i> =1.950(5), <i>g</i> _⊥ =2.459(3)				1/2	¹⁹⁵ <i>A</i> =0(5) ¹⁹⁵ <i>B</i> =135(5)	66Sim
					78	<i>g</i> =1.935(5), <i>g</i> _⊥ =2.51(2)					¹⁹⁵ <i>A</i> <28 ¹⁹⁵ <i>B</i> =135(10)	63Sro1
e ⁻	**)	1/2 (2)	10	10	55	1.930	1.911					63Sro2, 66Tak2, 67Tak

*) Paramagnetic center. **) Oxygen vacancy.

^{a)} Temperature dependence of *D*² in the tetragonal phase is linear [65Ves].^{b)} Forbidden transition lines ($\Delta M=\pm 1$, $\Delta m=\pm 1$) are observed. [63Ode, 64Iku].Forbidden transition lines ($\Delta M=\pm 1$, $\Delta m=\pm 2$) are observed. [65Iku, 66Iku].^{c)} Temperature dependence of ⁵⁵*A*. [67Zda2].^{d)} Fe³⁺ spectra are studied with a d.c. bias electric field near transition temperature from cubic to tetragonal phase and from tetragonal to orthorhombic phase. [63Sak2, 64Ell].^{e)} Forbidden transition lines ($\Delta M=2, 3, 4, 5$) are observed in the rhombohedral phase. [64Sak].^{f)} Fe³⁺ spectra due to the oxygen vacancy; *g*_{||}≈2, *g*_⊥=6.0(1) at 77 K. [65Gai].^{g)} Hyperfine structure of an electron captured by an oxygen vacancy. [64Dan].¹⁾ Mn²⁺ ion takes the place of Ti⁴⁺ lattice site in ceramics, while it takes the place of Ba²⁺ in a single crystal.²⁾ Positive *a* is assumed.³⁾ Fe³⁺ spectra in a single-domain specimen.

Table 1A-10-030. BaTiO₃: Gd³⁺. Spin Hamiltonian parameters of Gd³⁺ substituting for Ba²⁺ ions in BaTiO₃ measured at GHz range [68Tak].

T [°C]	g -factor (isotropic)	FS [10 ⁻² m ⁻¹]	
152	1.992(3)		$b_{40} \approx 6$
27	1.992(3)	$b_{20} = -293.6(10)$	$b_{40} = 4.0(10)$
			$b_{44} = -2.0(10)$
-23	1.993(3)	$b_{20} = 267.3(10)$	$b_{40} = 2.8(10)$
		$b_{22} = 5.6(20)$	$b_{42} = 11.2(30)$
			$b_{44} = -10.2(30)$
-196	1.992	$b_{20} = 340$	$b_{40} = 2$

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