No. 1C-a25 $CaTiO_3$–$BaTiO_3$

1b	Phase diagram: Fig. 1C-a25-001; see also	55DeV
3a	Lattice constant: Fig. 1C-a25-002.	
b	Crystal structure: Table 1C-a25-001.	
5a	Dielectric properties: Figs. 1C-a25-003...1C-a25-005; see also	87Pan, 94Tiw
	Dielectric relaxation: Fig. 1C-a25-006, Fig. 1C-a25-007. Effect of external stress on dielectric constant: Fig. 1C-a25-008.	
6b	Thermal conductivity: Fig. 1C-a25-009.	
7a	Piezoelectricity: Table 1C-a25-002.	

Table 1C-a25-001. $(Ba_{0.88}Ca_{0.12})TiO_3$. Structural parameters by profile analysis of neutron scattering data [91Tiw].

Parameter	semiwet	dry
$a = b$ [Å]	3.9735(3)	3.9842(3)
c [Å]	4.0120(5)	4.0255(5)
Ba, Ca(0, 0, 0)		
B [Å^2]	0.32(6)	0.31(7)
N	0.88, 0.12(1)	0.88, 0.08(1)
Ti, Ca(0.5, 0.5, z)		
z	0.520(4)	0.496(5)
B [Å^2]	0.17(6)	0.30(7)
N	1.00(1), 0.00(1)	0.96(1), 0.04(1)
O(0.5, 0.5, z)		
z	–0.020(4)	–0.031(3)
B [Å^2]	0.34(6)	0.50(7)
N	1.00(1)	0.96(1)
O(0, 0.5, z)		
z	0.476(3)	0.478(5)
B [Å^2]	0.29(2)	0.28(2)
N	2.00(2)	1.92(2)
Atomic distribution	$Ba_{0.88}Ca_{0.12}Ti_{1.00}Ca_{0.00}O_3$	$Ba_{0.88}Ca_{0.08}Ti_{0.96}Ca_{0.04}O_{2.88}$
R_p	2.65	2.56
R_{wp}	3.40	3.30
R_B	1.17	1.38

The scattering lengths used for Ba, Ca, Ti and O were 5.25, 4.90, –3.438 and 5.805 fm, respectively. Space group: P4mm. B: Isotropic temperature factor. N: Site occupancy.
R_p, R_{wp}, R_B: Reliability factors conventionally used in neutron powder diffraction structure analysis; see the original paper.

Table 1C-a25-002. $(Ba_{1-x}Ca_x)TiO_3$ (ceramics). Piezoelectric properties [57Ber].

x	ρ $[\cdot 10^3\,kgm^{-3}]$	ρ_X $[\cdot 10^3\,kgm^{-3}]$	d_{31} $[\cdot 10^{-12}\,CN^{-1}]$	d_{33} $[\cdot 10^{-12}\,CN^{-1}]$	$-d_{33}/d_{31}$	Porosity $(1-(\rho/\rho_X))$
0	5.85	6.017	–97.5	229	2.35	0.028
0.05	5.70	5.85	–66.6	167	2.51	0.026
0.07	5.68	5.80	–58.0	150	2.58	0.021
0.09	5.65	5.74	–52.1	139	2.67	0.016
0.12	5.55	5.66	–43.4	124.5	2.88	0.019

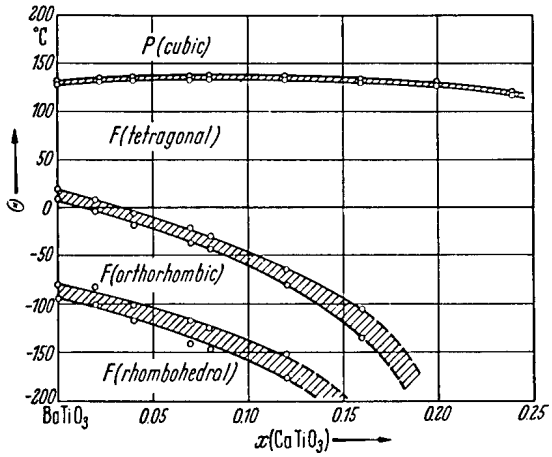

Fig. 1C-a25-001. $(Ba_{1-x}Ca_x)TiO_3$. Θ vs. x [61Mit]. Shaded areas represent temperature hysteresis regions.

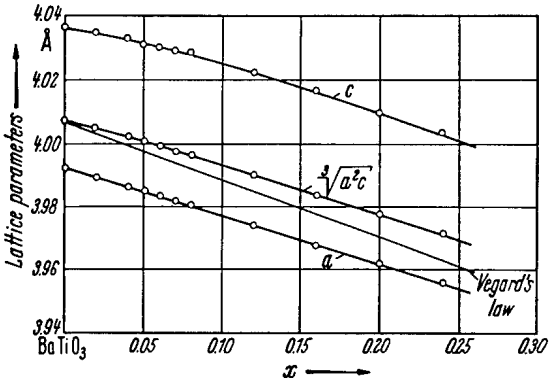

Fig. 1C-a25-002. $(Ba_{1-x}Ca_x)TiO_3$. *a*, *c*, $\sqrt[3]{a^2c}$ vs. x [61Mit].

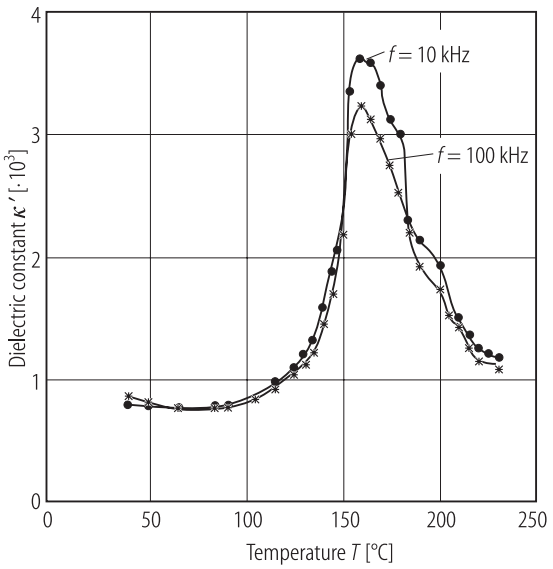

Fig. 1C-a25-003. $(Ba_{0.84}Ca_{0.16})TiO_3$ (crystal). κ' vs. T [94Bal]. Parameter: f.

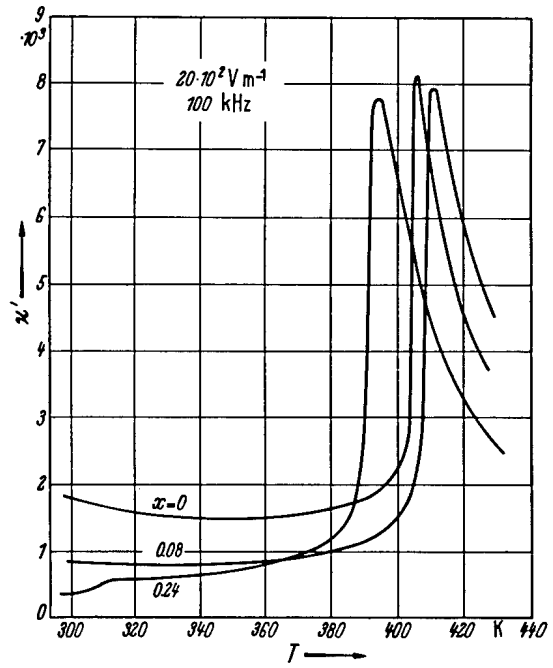

Fig. 1C-a25-004. $(Ba_{1-x}Ca_x)TiO_3$ (ceramics). κ' vs. *T* [61Mit]. Parameter: x. *f* = 100 kHz.

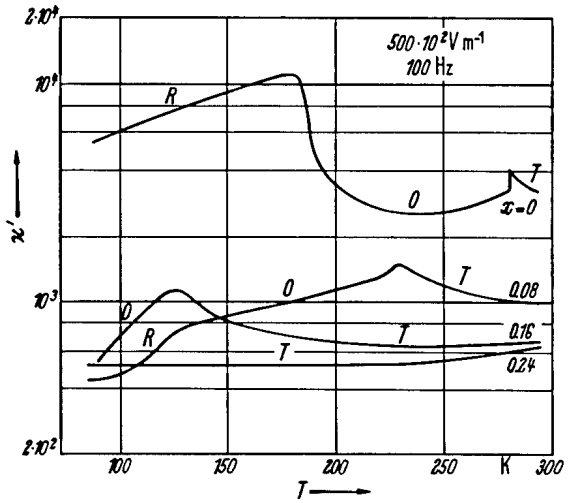

Fig. 1C-a25-005. $(Ba_{1-x}Ca_x)TiO_3$ (ceramics). κ' vs. T [61Mit]. Parameter: x. f = 100 Hz. T: tetragonal, O: orthorhombic, R: rhombohedral.

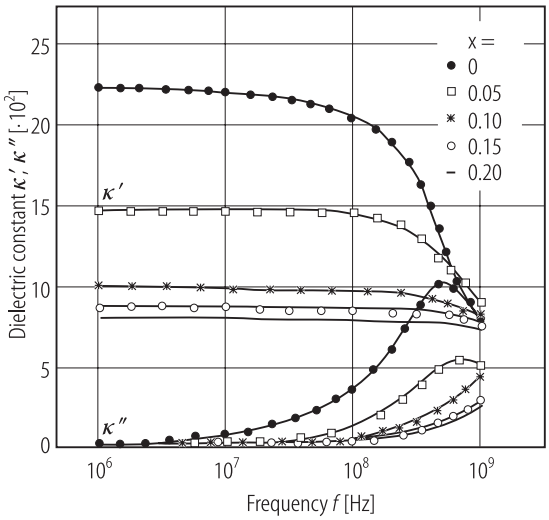

Fig. 1C-a25-006. $(Ba_{1-x}Ca_x)TiO_3$ (ceramics). κ', κ'' vs. f [92Kaw]. Parameter: x. $T \approx$ RT.

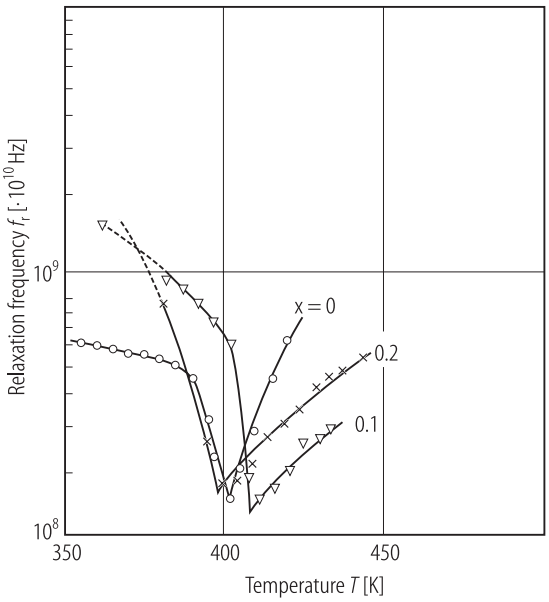

Fig. 1C-a25-007. $(Ba_{1-x}Ca_x)TiO_3$ (ceramics). f_r vs. T [92Kaw]. Parameter: x. f_r: dielectric relaxation frequency.

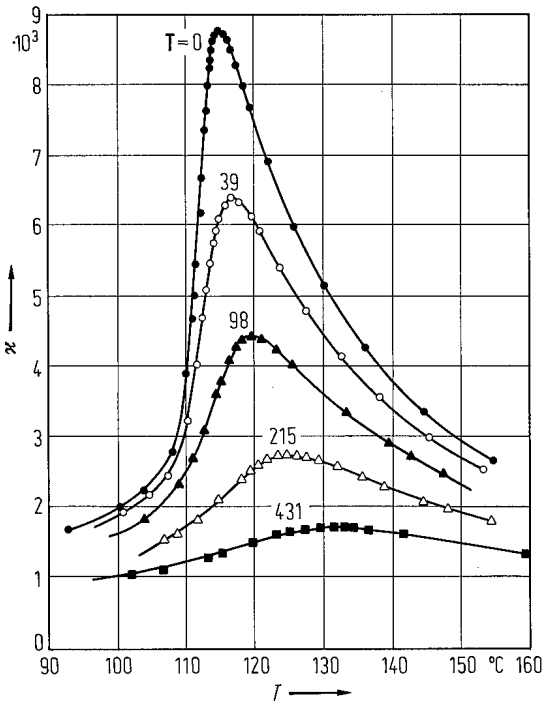

Fig. 1C-a25-008. $(Ba_{0.92}Ca_{0.08})TiO_3$ (ceramics). κ vs. T [78Fri]. Parameter: **T**. **T**: external stress in 10^6 Pa. f = 10 kHz.

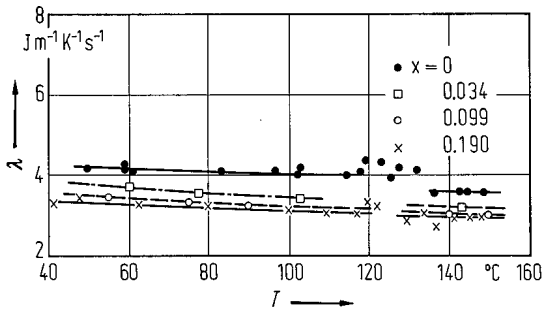

Fig. 1C-a25-009. $(Ba_{1-x}Ca_x)TiO_3$ (ceramics). λ vs. T [63Glo]. Parameter: x. λ: thermal conductivity.

References

55DeV DeVries, R.C., Roy, R.: J. Am. Ceram. Soc. **38** (1955) 142.

57Ber Berlincourt, D., Krueger, H.H.A.: Phys. Rev. **105** (1957) 56.

61Mit Mitsui, T., Westphal, W.B.: Phys. Rev. **124** (1961) 1354.

63Glo Glower, D.D., Wallace, D.C.: J. Phys. Soc. Jpn. **18** (1963) 679.

78Fri Fritz, I.J.: J. Appl. Phys. **49** (1978) 788.

87Pan Pandey, D., Tiwari, V.S., Singh, T.B., Pandey, L., Parkash, O., Ramachandrarao, P.: Phase Transitions **9** (1987) 11.

91Tiw Tiwari, V.S., Pandey, D., Krishna, P.S.K., Chakravarthy, R., Dasannacharya, B.A.: Physica B **174** (1991) 112.

92Kaw Kawazoe, T., Satoh, K., Hayashi, I., Mori, H.: J. Lightwave Technol. **10** (1992) 51; erratum: **10** (1992) 704.

94Bal Balakuma, S., Ilangovan, R., Subramanian, C., Pamasany, P.: Ferroelectrics **158** (1994) 115.

94Tiw Tiwari, V.S., Pandey, D.: J. Am. Ceram. Soc. **77** (1994) 1819.