No. 1B-c9 $Pb(Sc_{1/2}Nb_{1/2})O_3$
(M = 324.1)

1a Ferroelectricity in $Pb(Sc_{1/2}Nb_{1/2})O_3$ was discovered by Smolenskii et al. in 1959. 59Smo

b

phase	II	I
state	F	P
crystal system	rhombohedral	cubic
Θ [°C]	90	

68Ten

2a Crystal growth: melting method [a]), flux method ($PbO–B_2O_3$) [b]) [c]). [a])59Smo [b])70Fes [c])83Smo

3a a = 4.0955 Å, α = 89.42° at RT. 95Chu
Crystal structure analyses using high resolution neutron time of flight powder diffraction method were made based on the space group $Pm\bar{3}m$ in the paraelectric state and R3m in the ferroelectric state: Table 1B-c9-001.

4 Thermal distortion: Fig. 1B3–c9–001.

5a Dielectric constant: Figs. 1B-c9-002...1B-c9-009.
$d\Theta_{I–I}/dp$ = – 43 K/MPa for ordered specimen,
$d\Theta_{I–I}/dp$ = – 45 K/MPa for disordered specimen. 90Yas

c Spontaneous polarization: Fig. 1B-c9-010.

7a Piezoelectricity: Table 1B-c9-003.

9a Birefringence: Fig. 1B-c9-011, Fig.1B-c9-012.
Infrared spectrum: Fig. 1B-c9-013.

e Nonlinear optical property: Fig. 1B-c9-014, Fig. 1B-c9-015.

11 Electrical conductivity: $\sigma = 1.7...3.3 \cdot 10^{-10}\ \Omega^{-1}m^{-1}$ at RT. 70Fes

Table 1B-c9-001. $Pb(Sc_{1/2}Nb_{1/2})O_3$. Refined structural parameters for the cubic phase I at 400 K (**a**) and rhombohedral phase II at 200 K (**b**) [95Kni]. Fractional coordinates of atoms refined by the high resolution neutron time-of-flight powder diffraction method. B_{ij} is defined by Eq. (a) in Introduction.

(**a**) Space group: $Pm\bar{3}m$, a = 4.08153(1) Å.

Atom	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Sc/Nb	0.0000	0.0000	0.0000	0.95(2)	0.95(2)	0.95(2)	0.0	0.0	0.0
Pb	0.5000	0.5000	0.5000	4.15(3)	4.15(3)	4.15(3)	0.0	0.0	0.0
O	0.5000	0.0000	0.0000	0.90(4)	2.66(3)	2.66(3)	0.0	0.0	0.0

R_p = 5.8%, R_{wp} = 5.8%, R_{exp} = 4.3%, χ^2 = 1.81 for 21 variables.

(**b**) Space group: R3m, a = 4.08207(1) Å, α = 89.872(1)°.

Atom	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Sc/Nb	0.0343(2)	0.0343(2)	0.0343(2)	0.55(2)	0.55(2)	0.55(2)	0.0	0.0	0.0
Pb	0.5000	0.5000	0.5000	1.99(3)	1.99(3)	1.99(3)	–0.78(2)	–0.78(2)	–0.78(2)
O	0.5301(6)	0.0462(6)	0.0462(6)	1.12(4)	2.64(5)	2.64(5)	0.95(4)	0.95(4)	1.05(6)

R_p = 5.4%, R_{wp} = 5.2%, R_{exp} = 4.1%, χ^2 = 1.66 for 28 variables.

Table 1B-c9-002. $Pb(Sc_{1/2}Nb_{1/2})O_3$. Piezoelectric parameters [70Fes].

k_p	k_{33}	d_{33} [$\cdot 10^{-12}$ CN^{-1}]	d_{31} [$\cdot 10^{-12}$ CN^{-1}]
0.11...0.21	0.12	409	117

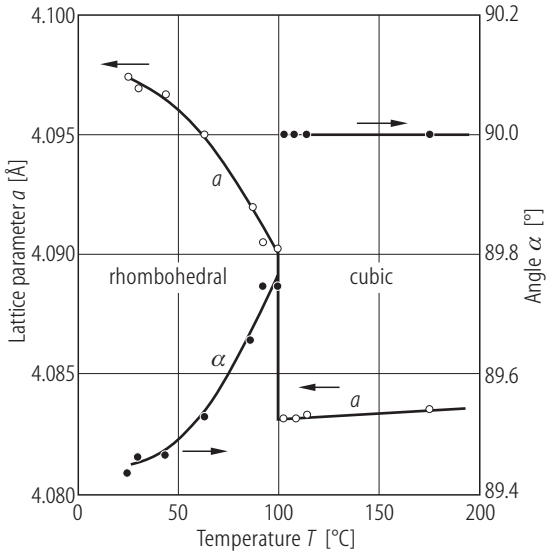

Fig. 1B-c9-001. $Pb(Sc_{1/2}Nb_{1/2})O_3$ (ceramics). *a*, α vs. *T* [95Chu].

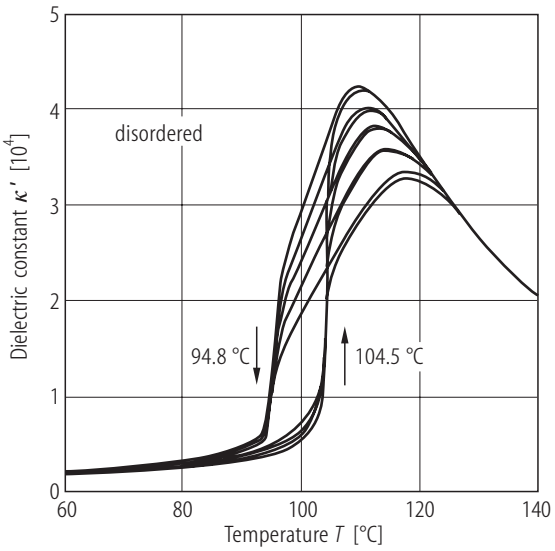

Fig. 1B-c9-002. $Pb(Sc_{1/2}Nb_{1/2})O_3$ (ceramics). κ' vs. T [95Chu]. f: 10^2, 10^3, 10^4, 10^5 and 10^6 Hz.

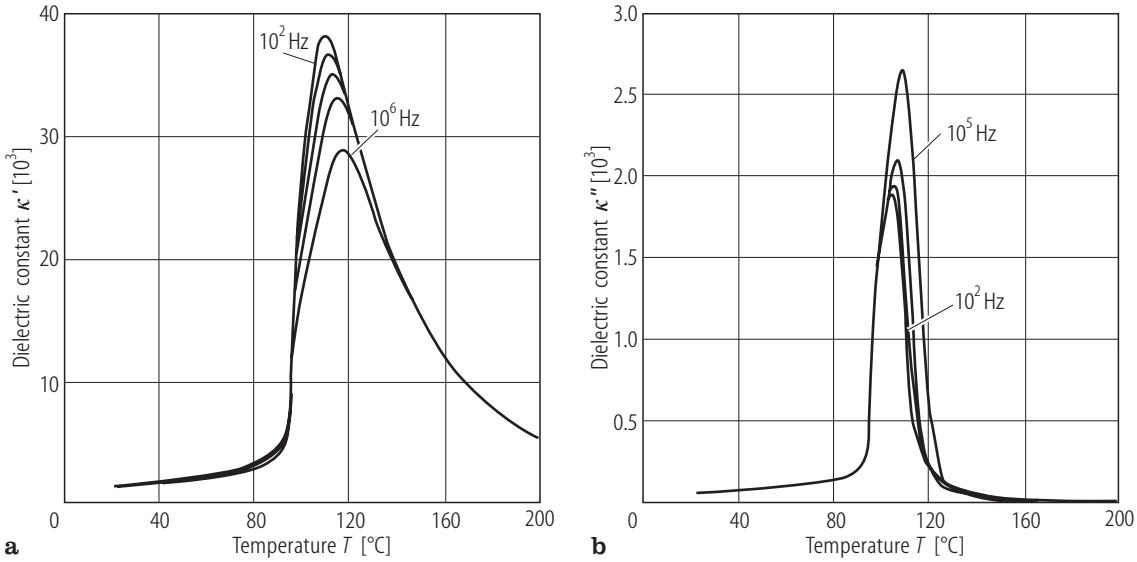

Fig. 1B-c9-003. $Pb(Sc_{1/2}Nb_{1/2})O_3$ (ceramics). κ', κ'' vs. T [95Chu]. f: 10^2, 10^3, 10^4, 10^5 and 10^6 Hz.

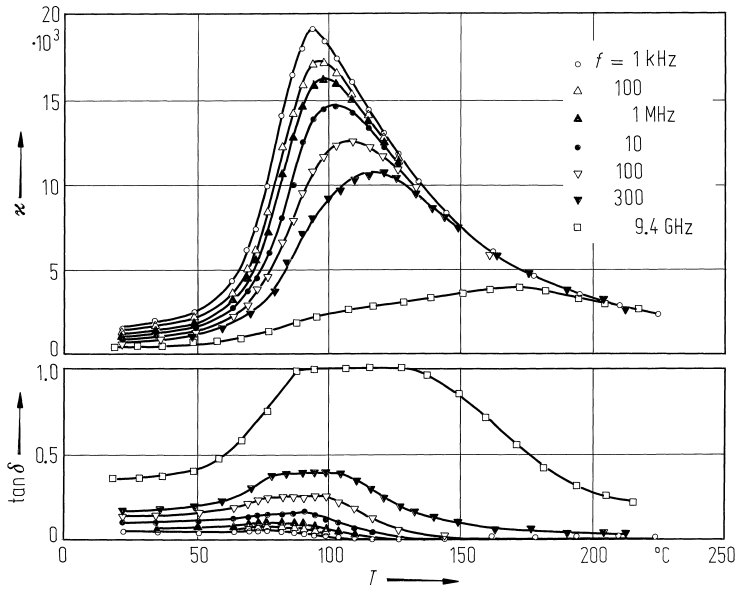

Fig. 1B-c9-004. $Pb(Sc_{1/2}Nb_{1/2})O_3$ (ceramics). κ, $\tan\delta$ vs. T [84Ker]. Parameter: f.

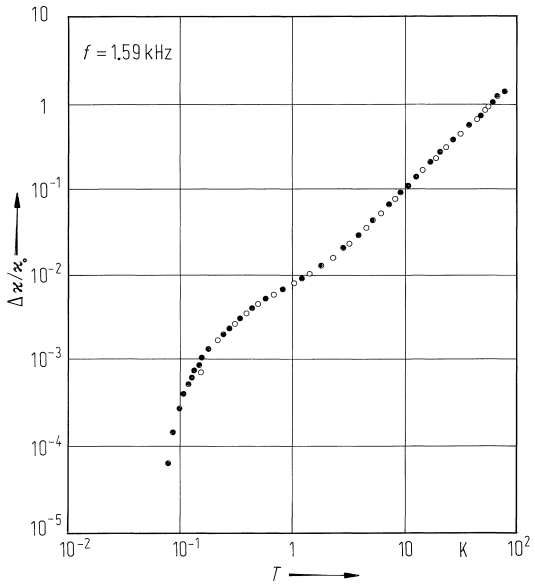

Fig. 1B-c9-005. $Pb(Sc_{1/2}Nb_{1/2})O_3$ (ceramics). $\Delta\kappa/\kappa_0$ vs. T [87Zim]. f = 1.59 kHz. $\Delta\kappa = \kappa'(T) - \kappa_0$. κ_0: κ' at 0.07 K. Full circles: poled specimen. Open circles: depoled specimen.

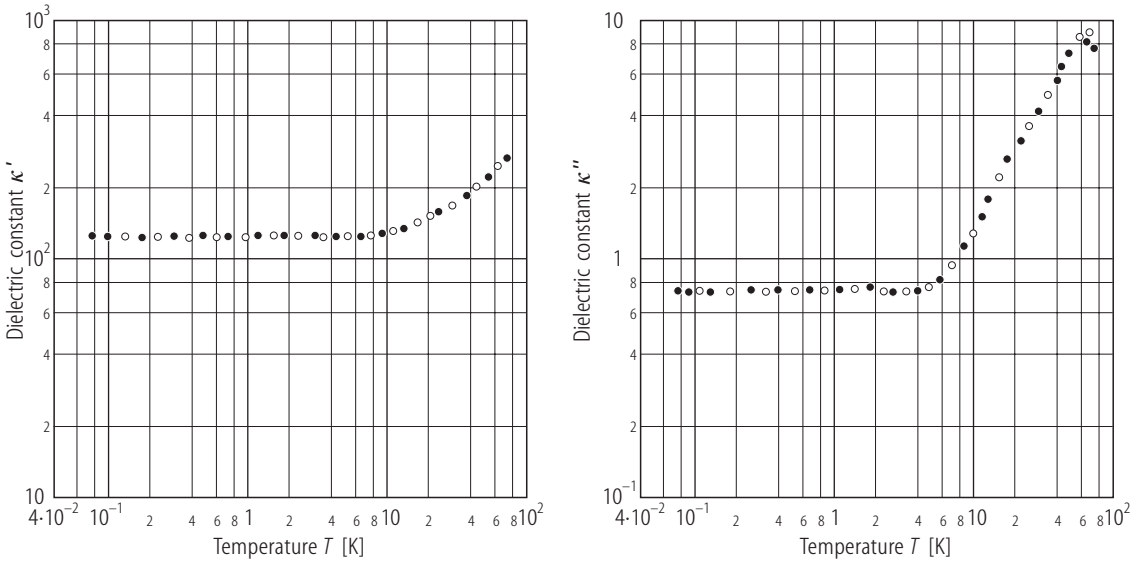

Fig. 1B-c9-006. $Pb(Sc_{1/2}Nb_{1/2})O_3$ (ceramics). κ', κ'' vs. T [87Zim]. Full circles: poled sample. Open circles: depoled sample.

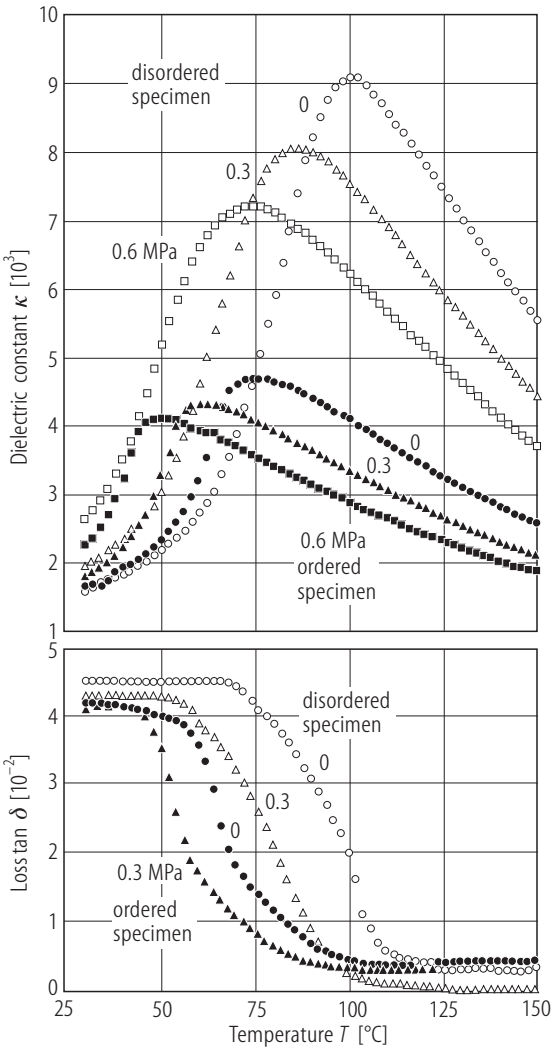

Fig. 1B-c9-007. $Pb(Sc_{1/2}Nb_{1/2})O_3$ (ceramics). κ, $\tan\delta$ vs. T [90Yas]. Parameter: hydrostatic pressure. Ordered specimen: specimen with ordered distribution of Sc and Nb at octahedral sites, disordered specimen: specimen with disordered distribution. f = 100 kHz.

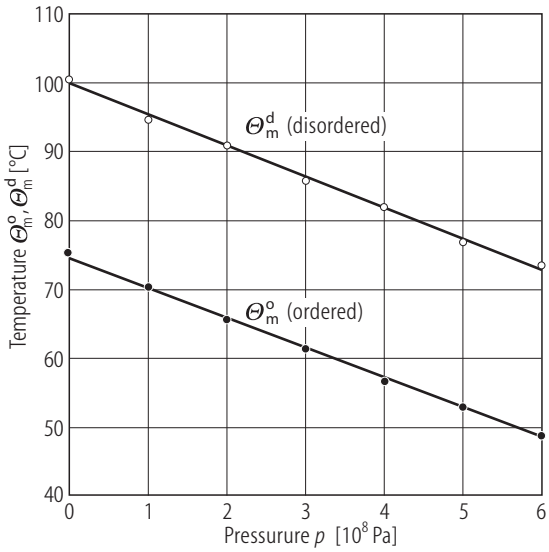

Fig. 1B-c9-008. $Pb(Sc_{1/2}Nb_{1/2})O_3$ (ceramics). Θ_m^o, Θ_m^d vs. p [89Yas]. Θ_m^o, Θ_m^d: the temperatures at which κ has its maximum for ordered (s = 0.8) and disordered samples, respectively. s: order parameter.

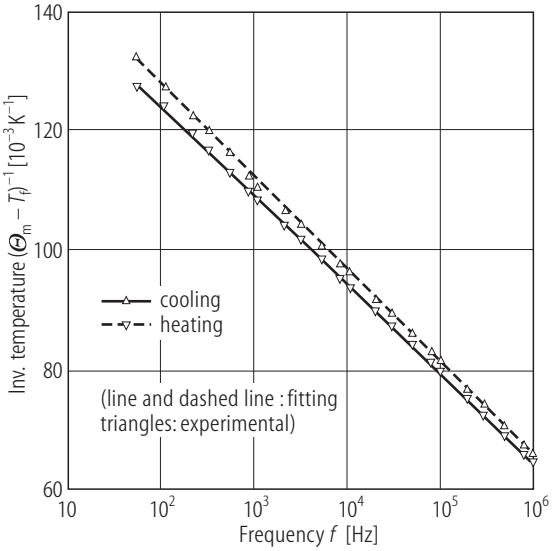

Fig. 1B-c9-009. $Pb(Sc_{1/2}Nb_{1/2})O_3$ (ceramics). $1/(\Theta_m - T_f)$ vs. f [95Chu]. Θ_m: the temperature at which κ has its maximum. T_f: static freezing temperature. The Vogel-Fulcher relationship $f = f_0 \exp\{E_a/[\kappa(\Theta_m - T_f)]\}$: $f_0 = 4.4 \cdot 10^9$ Hz, $E_a = 0.014$ eV, $T_f = 376$ K.

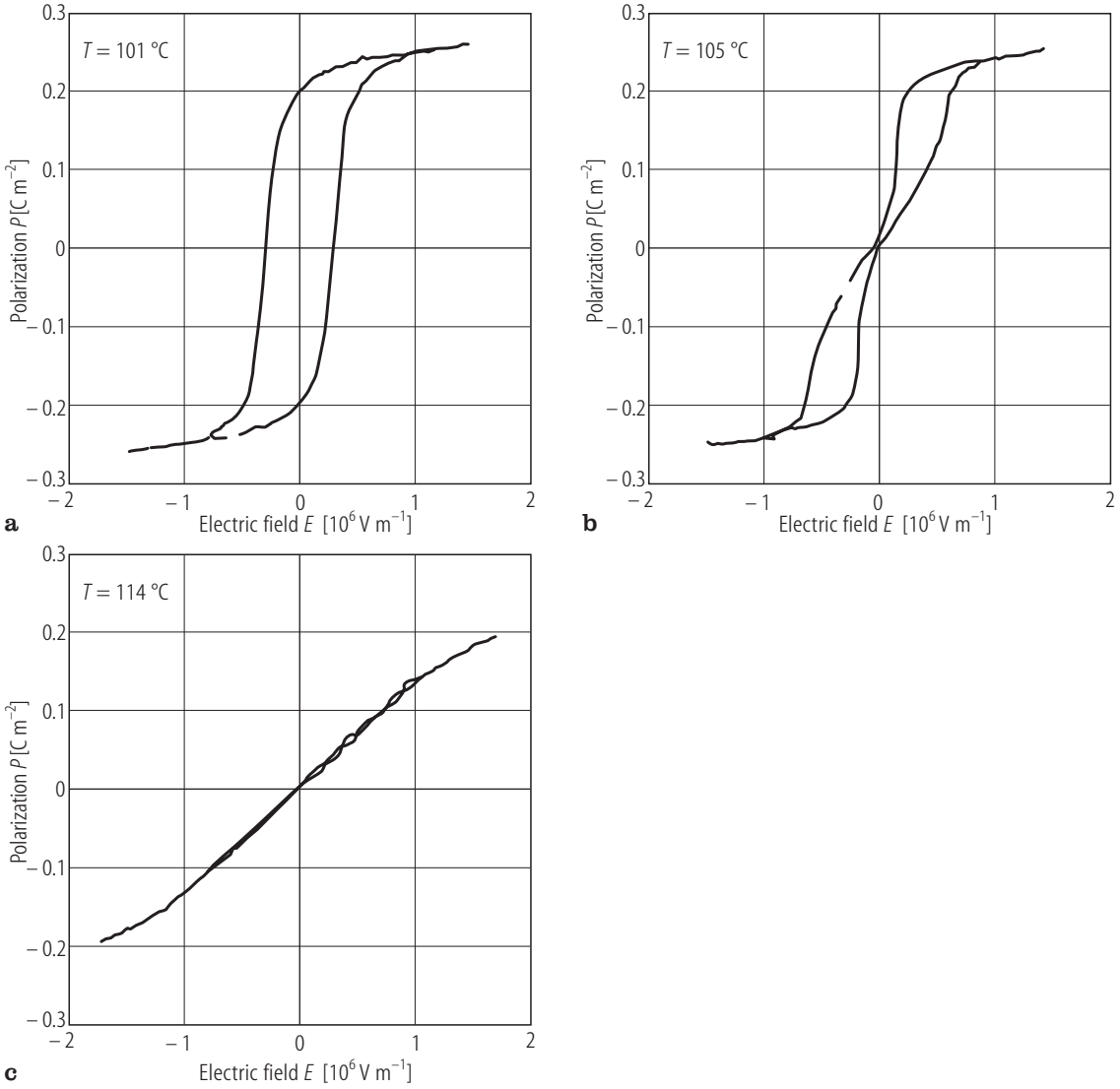

Fig. 1B-c9-010. $Pb(Sc_{1/2}Nb_{1/2})O_3$ (ceramics). *P* vs. *E* [95Chu]. Parameter: (**a**) *T* = 101 °C, (**b**) *T* = 105 °C, (**c**) *T* = 114 °C.

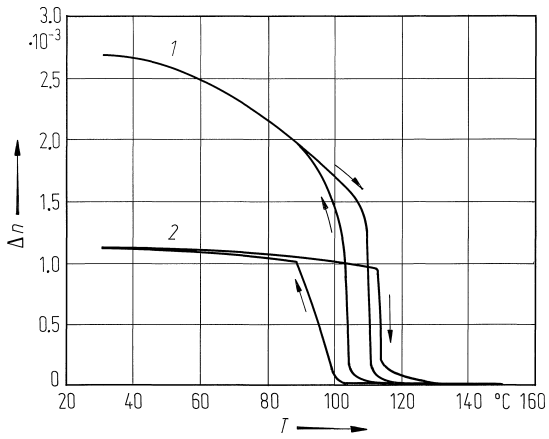

Fig. 1B-c9-011. $Pb(Sc_{1/2}Nb_{1/2})O_3$. Δn vs. T [81Set]. He-Ne laser light. Curve *1*: as grown. *2*: after 2 h at 1350 °C.

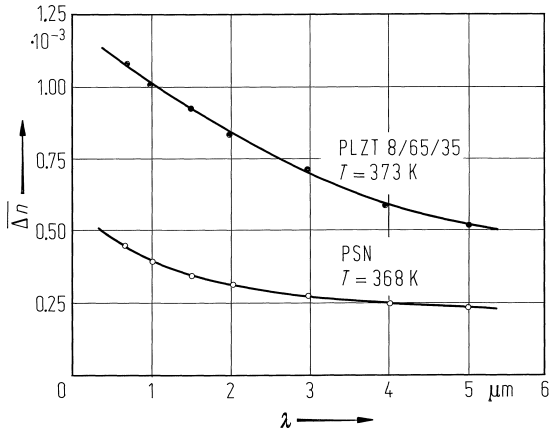

Fig. 1B-c9-012. $Pb(Sc_{1/2}Nb_{1/2})O_3$ (PSN), PLZT(8/65/35). $\overline{\Delta n}$ vs. λ [86Kni]. Δn: effective birefringence under electric field. Length is 1.5 mm, electrode separation is 1.5 mm, V = 1 kV.

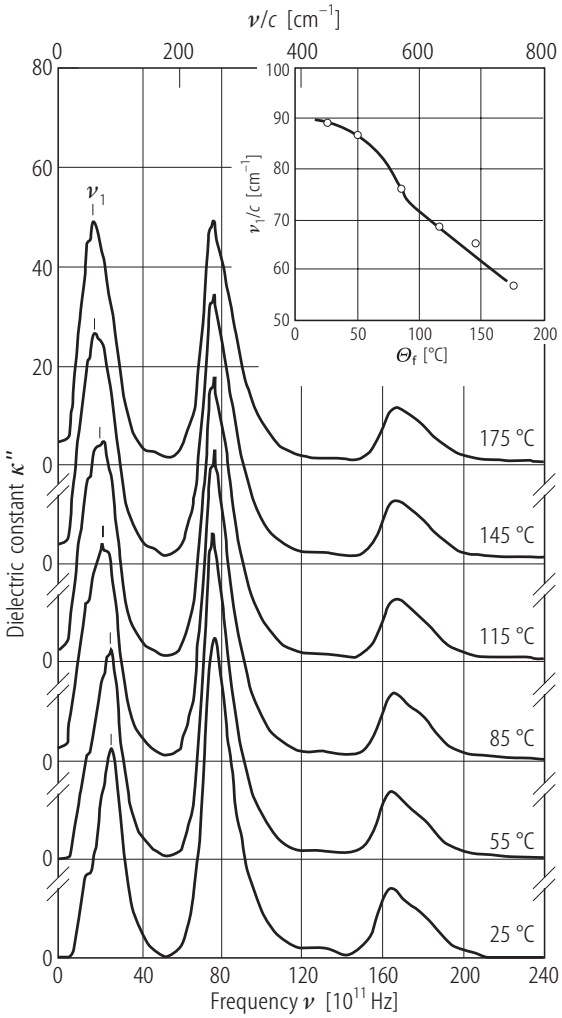

Fig. 1B-c9-013. $Pb(Sc_{1/2}Nb_{1/2})O_3$(ceramics). κ'' vs. ν [90Zel]. Parameter: T. The results were calculated from the infrared reflectivity. $\Theta_f \approx 90$ °C. Insert: ν_1/c vs. T. ν_1 is the lowest phonon mode frequency.

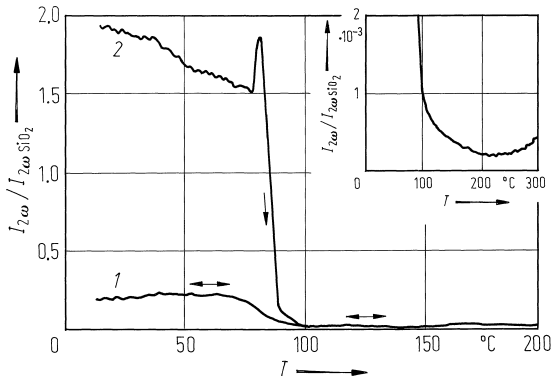

Fig. 1B-c9-014. $Pb(Sc_{1/2}Nb_{1/2})O_3$. $I_{2\omega}/I_{2\omega SiO_2}$ vs. T [80Lib]. $I_{2\omega}$: optical second harmonic intensity. $I_{2\omega SiO_2}$: $I_{2\omega}$ of SiO_2 standard. Curve *1:* polarized (at 20 °C, $E = 5 \cdot 10^2$ kVm^{-1}); *2*: depolarized. $\lambda = 1.06$ μm.

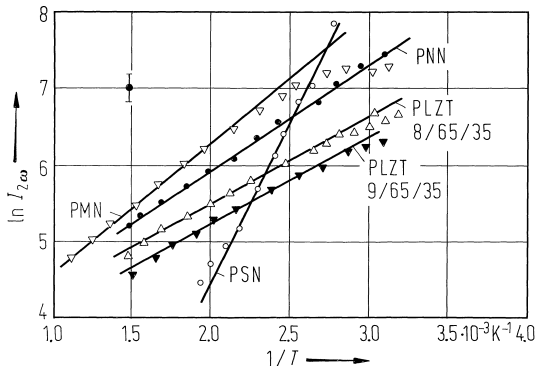

Fig. 1B-c9-015. $Pb(Sc_{1/2}Nb_{1/2})O_3$ (PSN), $Pb(Ni_{1/3}Nb_{2/3})O_3$ (PNN), $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN), PLZT. ln $I_{2\omega}$ vs. $1/T$ [81Lib]. $I_{2\omega}$: optical second harmonic intensity. $I_{2\omega}$ in arbitrary units. λ = 1.064 μm.

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