No. 1B-c11 $Pb(Fe_{1/2}Nb_{1/2})O_3$
(M = 329.6)

1a	Ferroelectricity in $Pb(Fe_{1/2}Nb_{1/2})O_3$ was discovered by Smolenskii et al. in 1958.		58Smo

	phase	III	II	I	
b	state	F, A_{magn}	F, P_{magn}	P, P_{magn}	62Bok
	crystal system	rhombohedral	rhombohedral	cubic	64Smo
	space group		$R3m - C_{3v}^5$	$Pm3m - O_h^1$	69Pla
	Θ [K]		143 (average)	387 (average) ≈393(1)	84Abd

2a	Crystal growth: flux method with PbO.	62Bok
3a	a = 4.0127(5) Å, α = 89.91(3)° at RT.	84Abd
b	Crystal structure: disordered perovskite; X-ray studies have not shown any ionic ordering in the octahedral sites of perovskite structure. The magnetic peak was found in the neutron diffraction experiments at 78 K. The effective magnetic moment of the Fe^{3+} ion was found to be 0.80(16) μ_B at 78 K from the calculation of the intensity of the (111) reflection, which is about 90% of the magnetic moment at 0 K. See Fig. 1B-c11-001.	64Smo
	The atomic structure of $Pb(Fe_{1/2}Nb_{1/2})O_3$ at RT was determined by micro electron diffraction, X-ray diffraction and powder neutron profile analysis methods: Tables 1B-c11-001...1B-c11-003.	69Kis
4	Thermal distortion: Fig. 1B-c11-002. Thermal expansion: Fig. 1B-c11-003.	
5a	Dielectric constants: Figs. 1B-c11-004...1B-c11-009.	
c	Spontaneous polarization and coercive field: Fig. 1B-c11-010, Fig. 1B-c11-011.	
7a	Piezoelectricity: Table 1B-c11-004. See also Fig. 1B-c11-012.	
8a	Elastic compliance: Fig. 1B-c11-013.	
9a	Optical absorption: Fig. 1B-c11-014.	
11	Electrical resistivity: Fig. 1B-c11-015.	
12	Magnetic susceptibility: Fig. 1B-c11-016. Magnetoresistance: see	74Ism
13b	ESR: Fig. 1B-c11-017.	
c	Mössbauer: Table 1B-c11-006. See also	68Bel
15a	Domain structure was observed by polarized light.	81Bru

Table 1B-c11-001. $Pb(Fe_{1/2}Nb_{1/2})O_3$. Displacements of ions [69Pla]. The displacements are given in fraction of the lattice parameter.

Method of investigation	Pb	Fe	Nb	O
Micro electron diffraction	0.000	0.004	0.004	0.017
X-ray diffraction	0.000	0.005	0.005	0.023

Table 1B-c11-002. Pb($Fe_{1/2}Nb_{1/2}$)O_3. Interatomic distances (electron diffraction data) [69Pla].

Distance	Without displacement of ions [Å]	With displaced ions [Å]
Pb–Fe	3.55	3.52
		3.58
Pb–Nb	3.55	3.52
		3.58
Pb–O	2.83	2.94
		2.73
Fe–O	2.11	2.06
		2.15
Nb–O	2.11	2.06
		2.15

Table 1B-c11-003. $Pb(Fe_{1/2}Nb_{1/2})O_3$. Atomic position parameters and unit cell parameters refined by powder neutron profile analysis with isotropic temperature parameters [84Abd]. The parameters *s* and *t* measure the fractional displacement of Pb and Fe/Nb, respectively, along the three fold axis, and *d* indicates a distortion of the oxygen octahedron. Based on the hexagonal cell (a_h, c_h) atomic position parameters are Pb: 0, 0, 1/4+*s*, Fe/Nb: 0, 0, *t*, and O: 1/6–2*e*–2*d*, 1/3–4*d*, 1/12. In the present case of R3m symmetry *e* is zero. ζ: octahedron strain defined by $\zeta = c_h / \sqrt{6}\, a_h - 1$. a_{pc}, α_{pc} and a_h, c_h are unit cell parameters of the pseudocubic and the hexagonal cells, respectively.

	T = –183°C	T = 25°C
s	0.0282(7)	0.0189(17)
t	0.0159(7)	0.0109(11)
d	–0.0017(11)	–0.0019(10)
ζ	0.0045	0.0019
α_{pc} [°]	89.828	89.927
a_{pc} [Å]	4.0112(6)	4.0101(10)
a_h [Å]	5.6600(6)	5.6676(10)
c_h [Å]	13.9262(25)	13.9087(51)

Table 1B-c11-004. $Pb(Fe_{1/2}Nb_{1/2})O_3$. Physical constants of hot-pressed ceramics at RT [93Yok].

Dielectric constants		Piezoelectric constants	
κ_{un} (unpoled)	2570	g_{31} [$\cdot 10^{-3}$ VmN^{-1}]	2.93
κ_{33}^{T} (poled)	2640	g_{33}	6.31
Loss tangents		Elastic compliance constants	
tan δ (unpoled)	0.0136	s_{11}^{E} [$\cdot 10^{-12}$ m^{2}N^{-1}]	12.0
tan δ (poled)	0.0157	s_{33}^{E}	12.3
Spontaneous polarization		s_{11}^{D}	11.8
P_s [Cm^{-2}]	0.113	s_{33}^{D}	11.3
Coercive field		Resistivity	
E_c [$\cdot 10^5$ Vm^{-1}]	4.6	ρ [$\cdot 10^9$ Ωm]	1.8
Electromechanical coupling factors		Thermal expansion coefficients	
k_{31}	0.128	β_{11} (unpoled) [$\cdot 10^{-6}$ K^{-1}]	1.06
k_{33}	0.266	β_{11} (poled)	2.86
k_p	0.161	Mechanical quality factor	
Piezoelectric constants		Q_M	240
d_{31} [$\cdot 10^{-12}$ C N^{-1}]	64.5		
d_{33}	145		

Table 1B-c11-005. $Pb(Fe_{1/2}Nb_{1/2})O_3$ (ceramics). Mössbauer parameters [94Wan].

Sample state	Ion state	Isomer shift [$\cdot 10^{-3}$ ms^{-1}]	Quadrupole splitting [$\cdot 10^{-3}$ ms^{-1}]	Linewidth [$\cdot 10^{-3}$ ms^{-1}]	Relative area [%]
undoped	Fe^{3+}	0.42	0.45	0.20	81
	Fe^{2+}	0.48	0	0.20	19
doped	Fe^{3+}	0.41	0.37	0.24	100

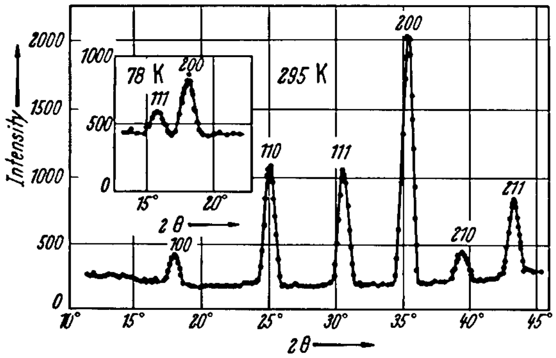


Fig. 1B-c11-001. $Pb(Fe_{1/2}Nb_{1/2})O_3$. Neutron diffraction patterns [65Dra].

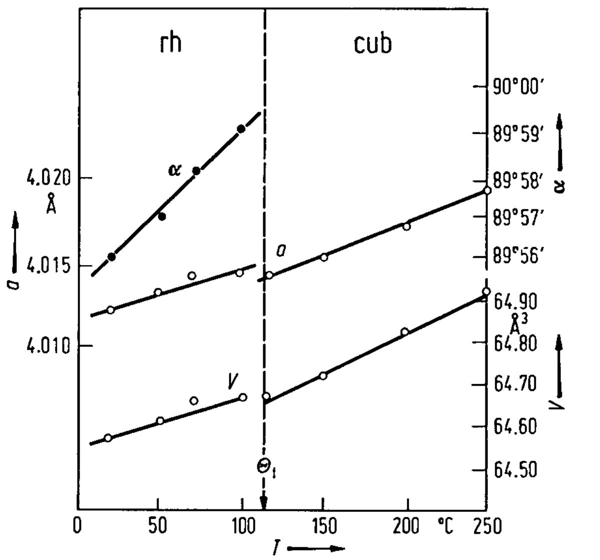


Fig. 1B-c11-002. $Pb(Fe_{1/2}Nb_{1/2})O_3$. *a*, *α*, *V* vs. *T* [68Ism]. *α*: rhombohedral angle.

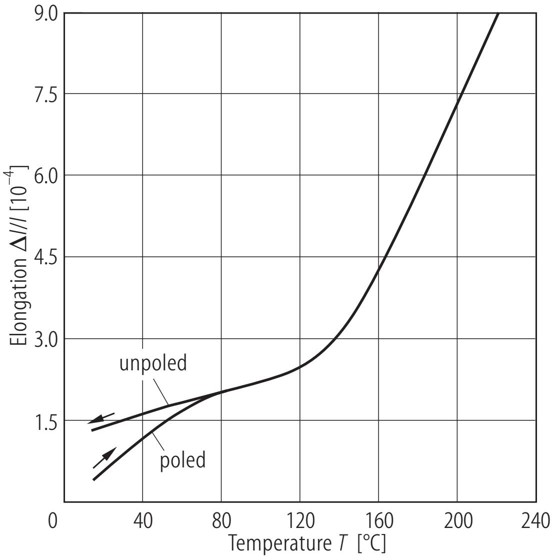


Fig. 1B-c11-003. $Pb(Fe_{1/2}Nb_{1/2})O_3$ (ceramics). $\Delta l/l$ vs. T [93Yok].

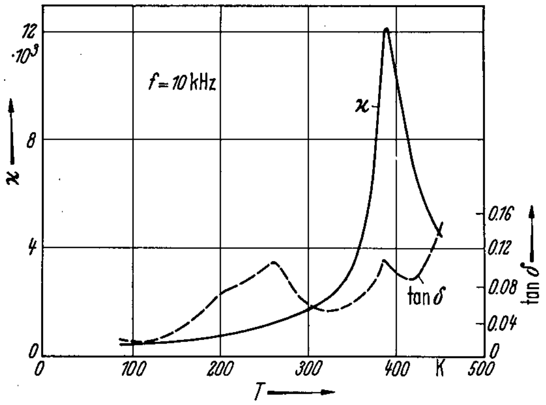


Fig. 1B-c11-004. $Pb(Fe_{1/2}Nb_{1/2})O_3$. κ, $\tan\delta$ vs. T [62Bok].
f = 10 kHz.

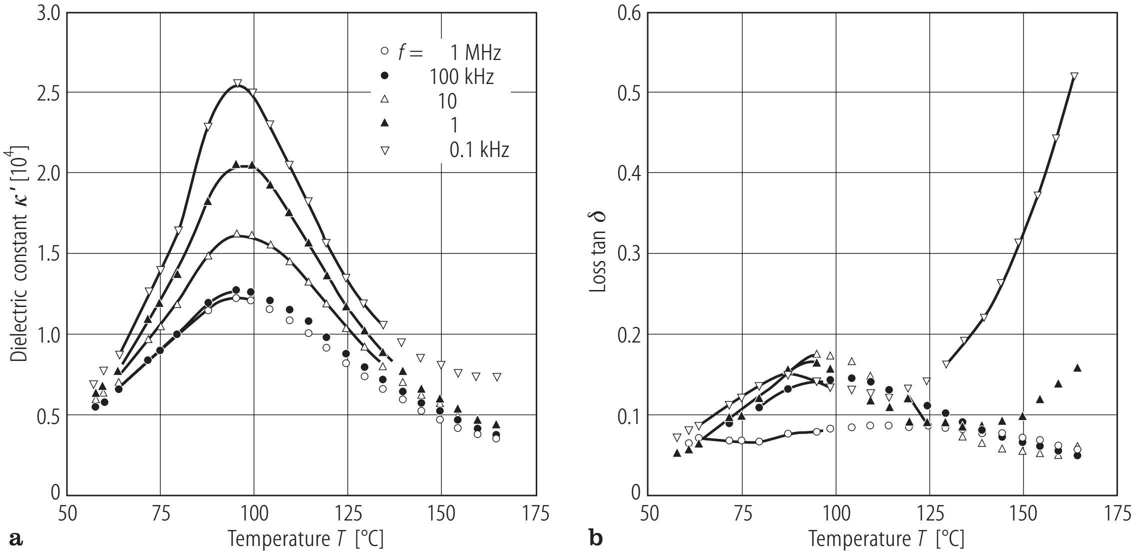


Fig. 1B-c11-005. $Pb(Fe_{1/2}Nb_{1/2})O_3$. κ' , tan δ vs. T [93Chi]. Parameter: f.

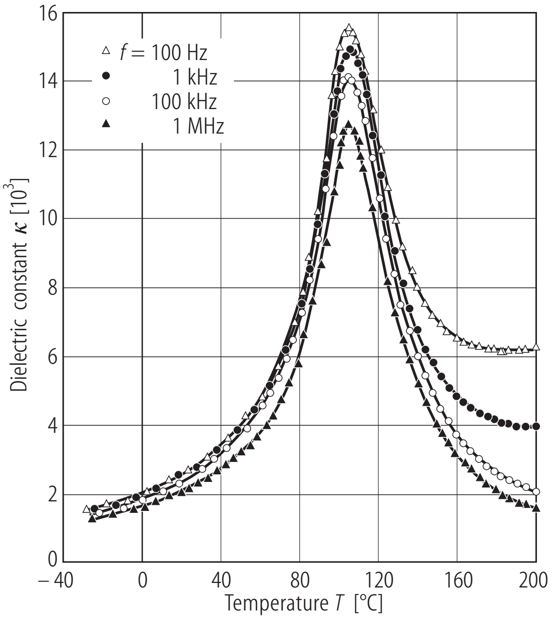


Fig. 1B-c11-006. $Pb(Fe_{1/2}Nb_{1/2})O_3$ (ceramics). κ vs. T [93Yok]. Parameter: f. Unpoled sample.

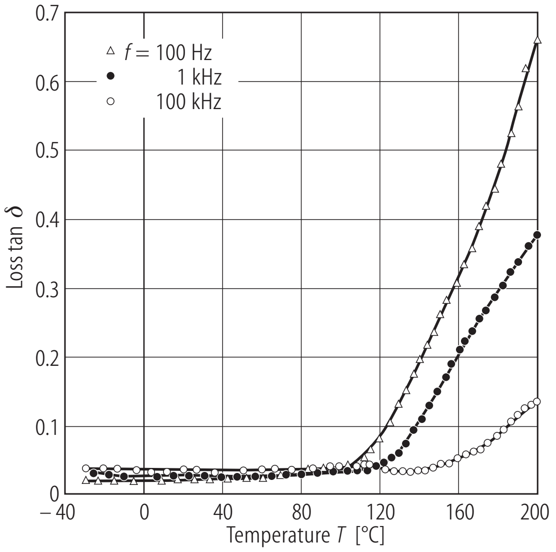


Fig. 1B-c11-007. $Pb(Fe_{1/2}Nb_{1/2})O_3$ (ceramics). tan δ vs. T [93Yok]. Parameter: f.

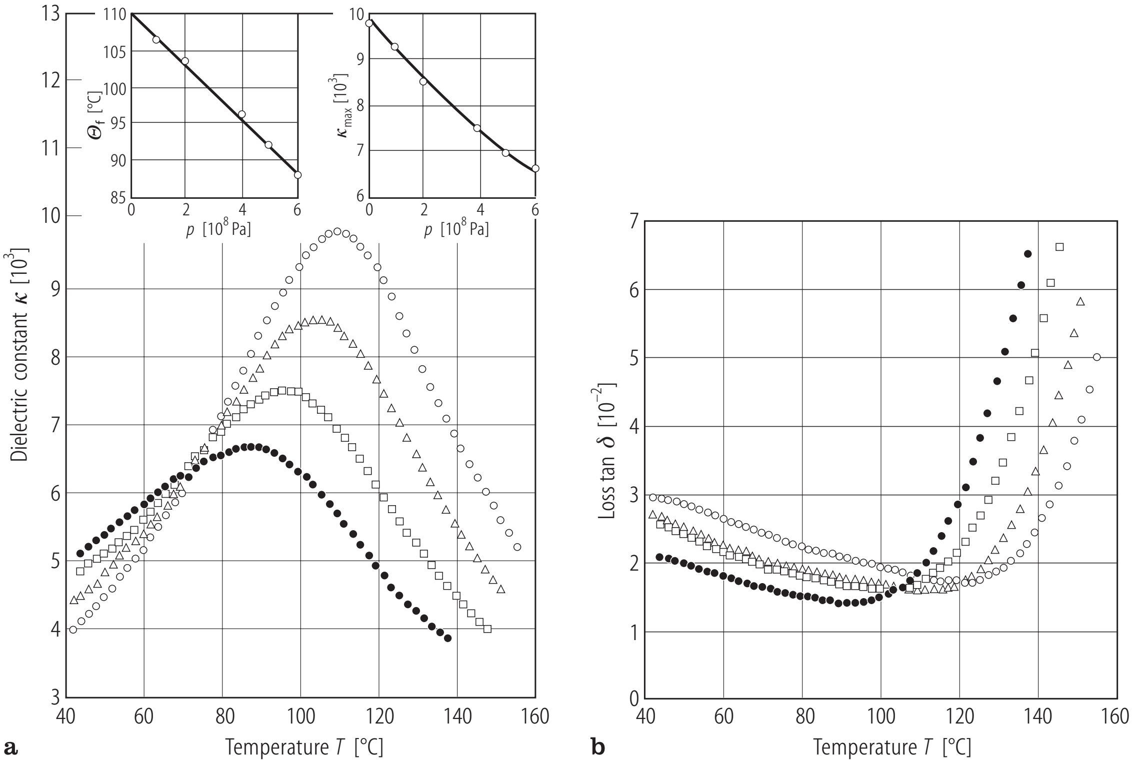


Fig. 1B-c11-008. $Pb(Fe_{1/2}Nb_{1/2})O_3$ (ceramics). κ, $\tan\delta$ vs. T [89Yas1]. Parameter: p. f = 100 kHz. Open circles: p = 0. Open triangles: $p = 2\cdot10^8$ Pa. Open squares: $p = 4\cdot10^8$ Pa. Full circles: $p = 6\cdot10^8$ Pa. Inserts shows Θ_f vs. p and κ_{max} vs. p. κ_{max}: maximum value of κ.

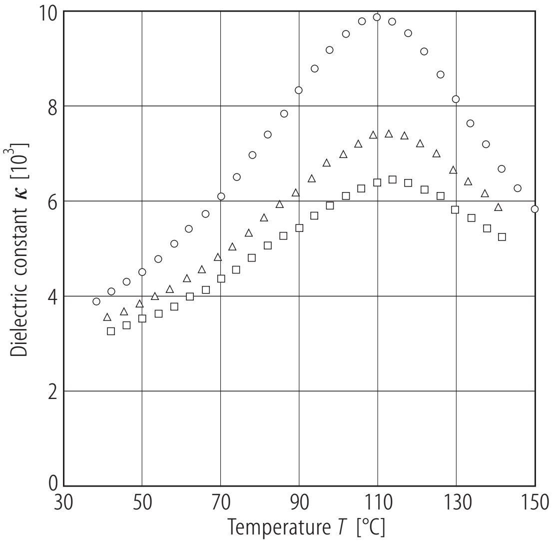


Fig. 1B-c11-009. $Pb(Fe_{1/2}Nb_{1/2})O_3$ (ceramics). κ vs. T [89Yas1]. Parameter: E_{bias}. f = 100 kHz. Open circles: E_{bias} = 0. Open triangles: $E_{bias} = 3.9\cdot10^2$ kVm^{-1}. Open squares: $E_{bias} = 6.6\cdot10^2$ kVm^{-1}.

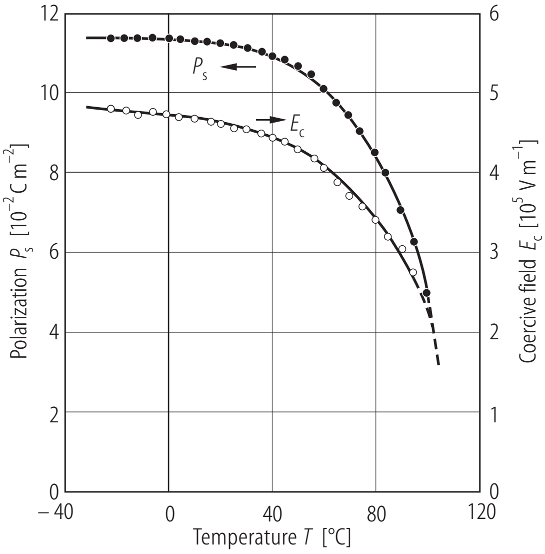


Fig. 1B-c11-010. $Pb(Fe_{1/2}Nb_{1/2})O_3$ (ceramics). P_s, E_c vs. T [93Yok].

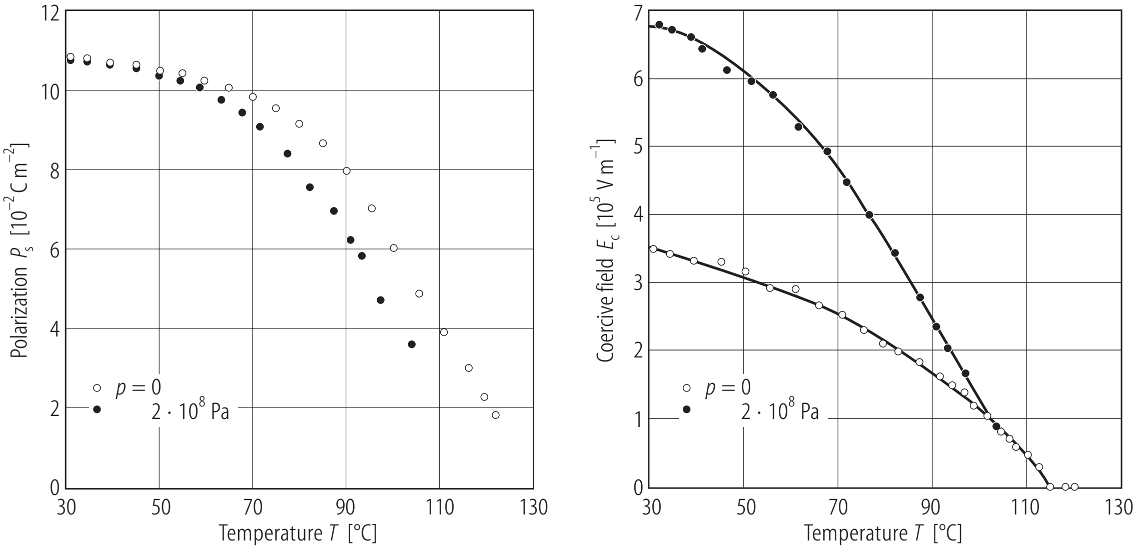


Fig. 1B-c11-011. $Pb(Fe_{1/2}Nb_{1/2})O_3$ (ceramics). P_s, E_c vs. T [89Yas2]. Parameter: p.

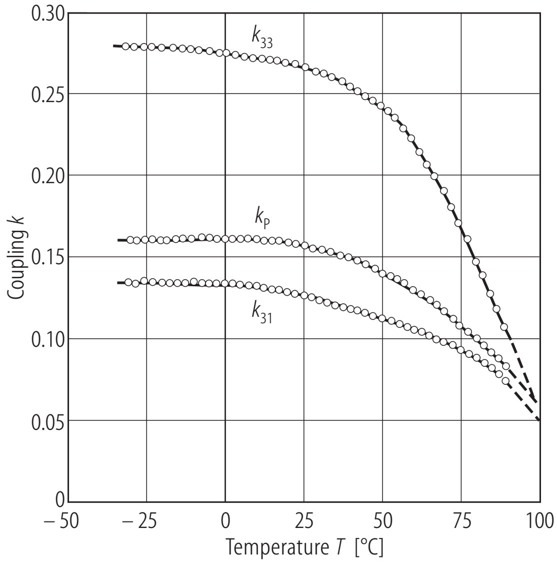
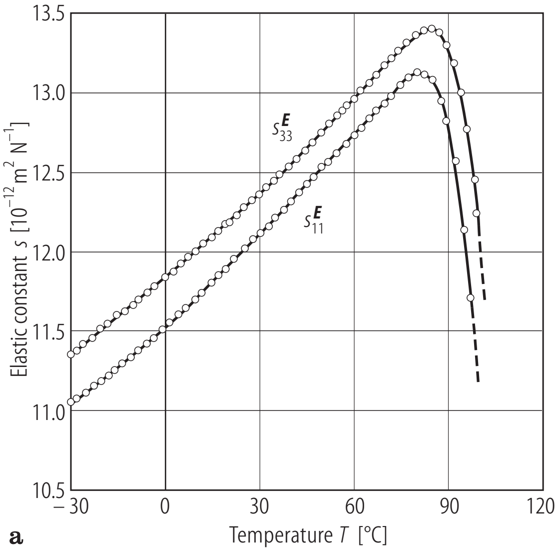


Fig. 1B-c11-012. $Pb(Fe_{1/2}Nb_{1/2})O_3$ (ceramics). k_{31}, k_p, k_{33} vs. T [93Yok].



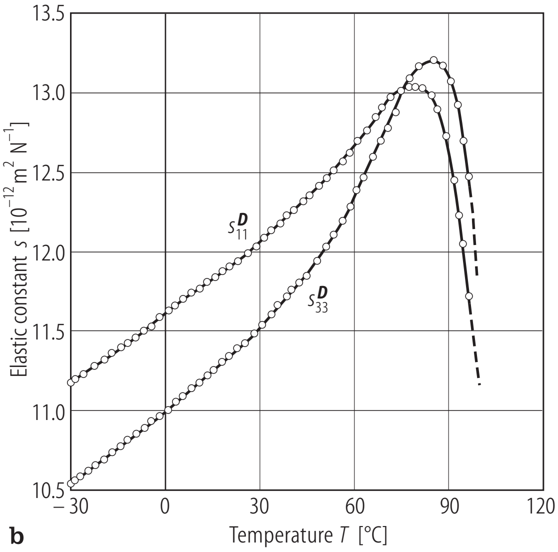


Fig. 1B-c11-013. $Pb(Fe_{1/2}Nb_{1/2})O_3$ (ceramics). s_{11}, s_{33} vs. T [93Yok].

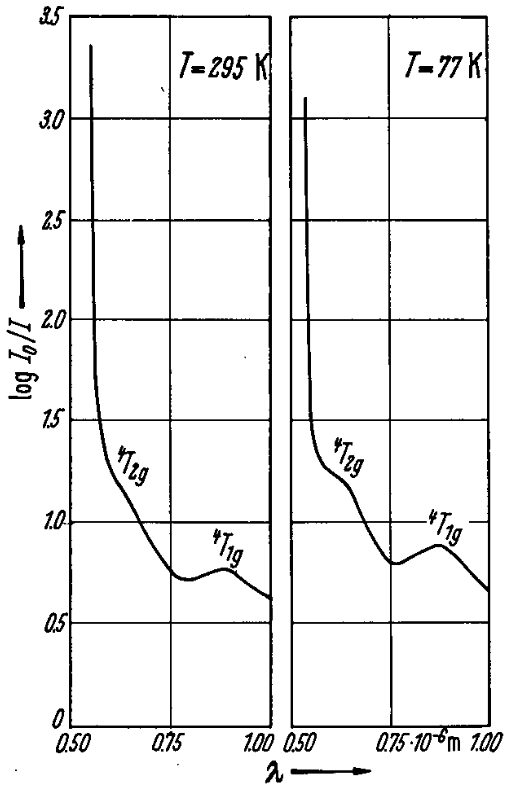


Fig. 1B-c11-014. $Pb(Fe_{1/2}Nb_{1/2})O_3$. Absorption spectrum. log (I_0/I) vs. λ [65Pis]. I_0: intensity of incident light, I: intensity of transmitted light. $^4T_{1g}$, $^4T_{2g}$ are excited Fe^{3+} levels in a cubic field.

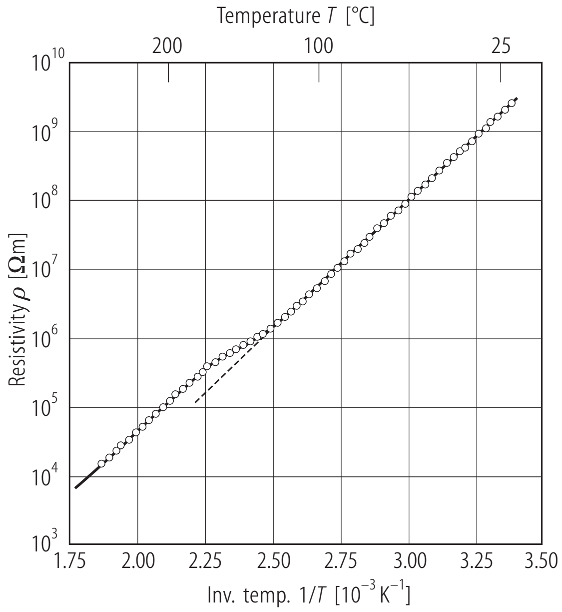


Fig. 1B-c11-015. $Pb(Fe_{1/2}Nb_{1/2})O_3$. ρ vs. $1/T$ [93Yok].

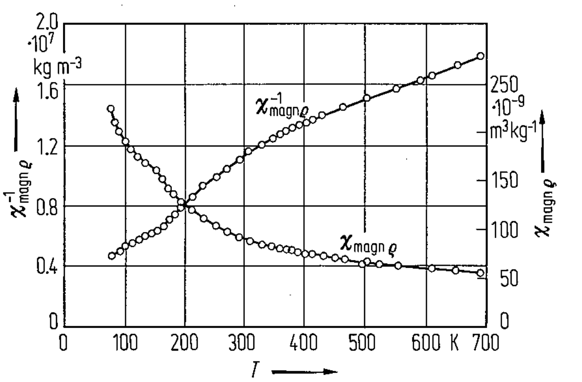


Fig. 1B-c11-016. $Pb(Fe_{1/2}Nb_{1/2})O_3$. $\chi_{magn\,\rho}$ and $\chi^{-1}_{magn\,\rho}$ vs. T [62Bok].

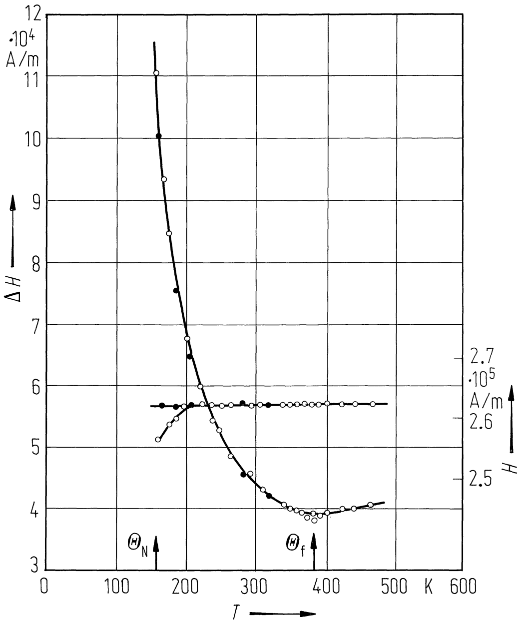


Fig. 1B-c11-017. $Pb(Fe_{1/2}Nb_{1/2})O_3$. *H*, Δ*H* vs. *T* [81Mar]. *H*: ESR resonance field for Fe^{3+} at 9.281 GHz. Δ*H*: ESR line width. Full circles: spherical shape sample. Open circles: cylindrical shape sample.

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