No. 1A-16 $PbHfO_3$, Lead hafnate

(M = 433.7)

1a A dielectric anomaly associated with a phase transition was observed, and the possibility of the antiferroelectricity was discussed by Shirane et al. in 1953. 53Shi

b

phase	III	II	I	
state	(A)		P	
crystal system	orthorhombic	rhombohedral	cubic	
space group	Pnam – D_{2h}^{16}	$R\bar{3}m$ – D_{3d}^{5} or $R\bar{3}c$ – D_{3d}^{6}	Pm3m – O_h^5	75Der
Θ [°C]	163		215	

2a Crystal growth: flux method with PbO. 75Der

3a a = 5.8572(5) Å, b = 11.689(1) Å, c = 4.0971(4) Å at RT. 75Der

b Crystal structure:
Atomic displacement from the cubic perovskite structure:
Δx_{Pb} = 0.211 Å, Δy_{Pb} = 0.023 Å, Δx_{Hf} = 0.082 Å, Δy_{Hf} = 0.012 Å (with accuracy of 0.006 Å); 83Kup
see also 79Zai
Effect of pressure on lattice parameter: Fig. 1A-16-001.
Crystal optical and crystallographic investigations of the first-order phase transitions have been carried out. 90Bal

4 Thermal expansion: Fig. 1A-16-002.
a = 5.854(1) Å, c = 7.145(2) Å (with hexagonal cell dimensions) at 450 K, 75Der
a = 4.1354(4) Å at 520 K;
see also 84Leo

5a Dielectric constant: Fig. 1A-16-003.
$C = 9.5 \cdot 10^4$ K (ceramics). 53Shi
Effect of p on κ: Fig. 1A-16-004.
Phase diagram in regard to p: Fig. 1A-16-005.
$[d\Theta_{II-I}/dp]_{p=0} = -10.0(10) \cdot 10^{-8}$ K Pa^{-1}, $C^* = 1.1 \cdot 10^{12}$ Pa, $p_0 = -12.8 \cdot 10^8$ Pa, T = 603 K 70Sam
($\kappa = C^*/(p-p_0)$ at constant T).

b Effect of electric field on dielectric property: Fig. 1A-16-006.

9a Optical absorption: see 83Yak

10a Raman scattering: Fig. 1A-16-007.
Pressure dependence of Raman spectrum: Fig. 1A-16-008.

11 Electrical conductivity: Fig. 1A-16-009.

12 Effect of magnetic field on Θ_{II-I}: see 84Ism

13c Mössbauer effect: Fig. 1A-16-010.
Perturbed γ–γ angular correlation: Fig. 1A-16-011, Fig. 1A-16-012; see also 73Ein, 73Kly

16 Twin structure: see 90Top

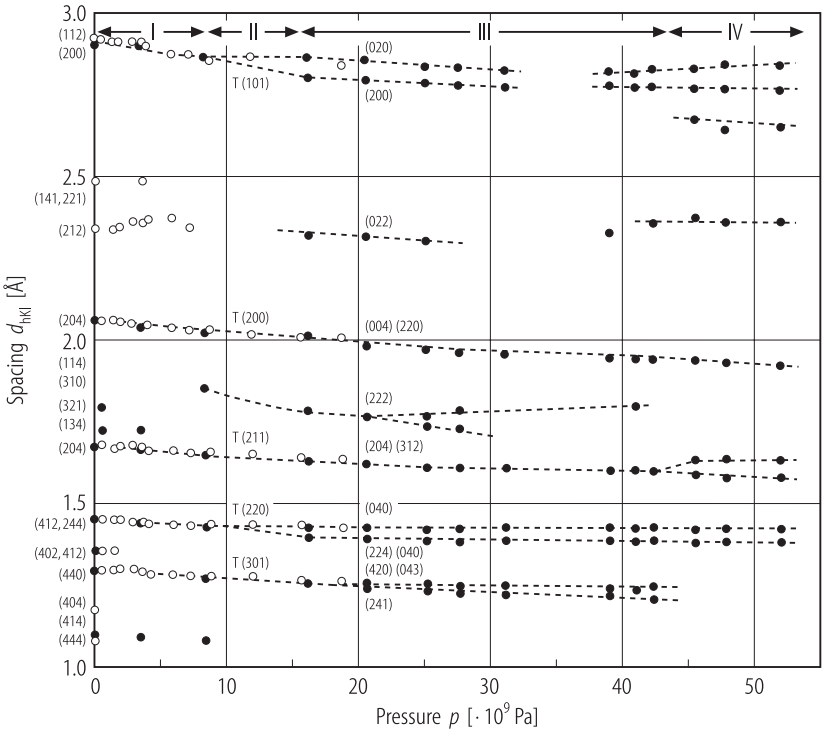

Fig. 1A-16-001. $PbHfO_3$. d_{hkl} vs. p [94Min].

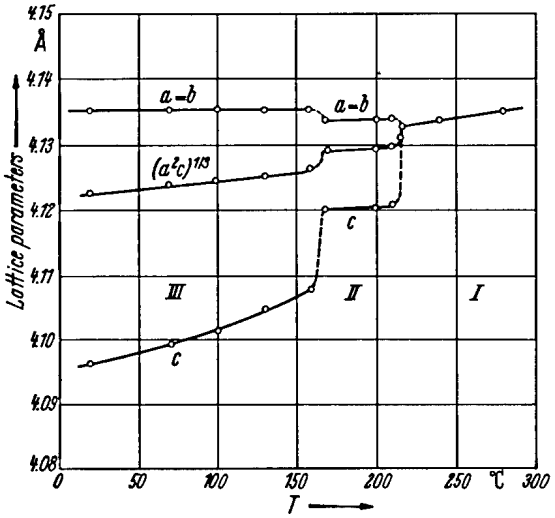

Fig. 1A-16-002. $PbHfO_3$. Lattice parameters a, c, $V^{1/3}$ vs. T [53Shi].

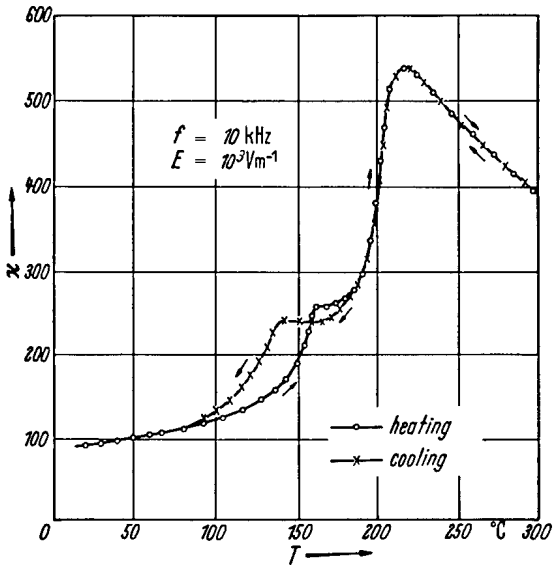

Fig. 1A-16-003. $PbHfO_3$ (ceramics). κ vs. T [53Shi].

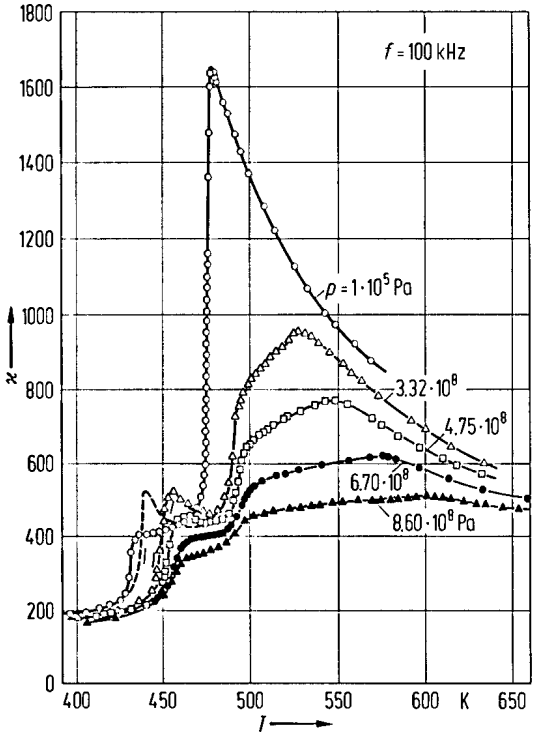

Fig. 1A-16-004. $PbHfO_3$ (ceramics). κ vs. T [70Sag]. Parameter: p.

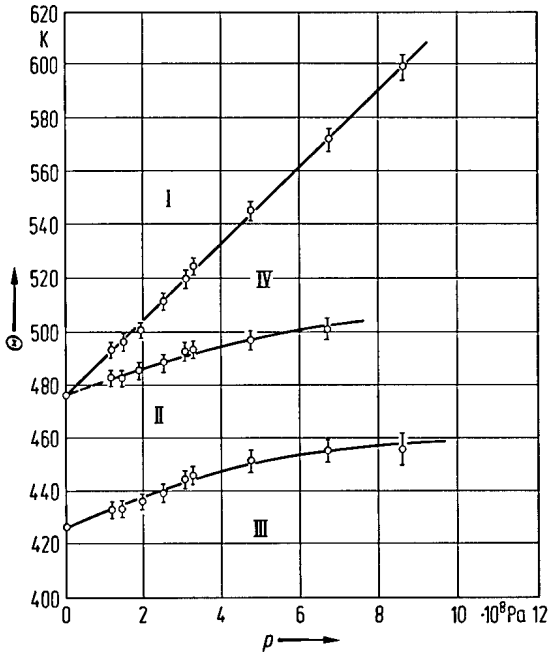

Fig. 1A-16-005. $PbHfO_3$. Θ vs. p [70Sag].

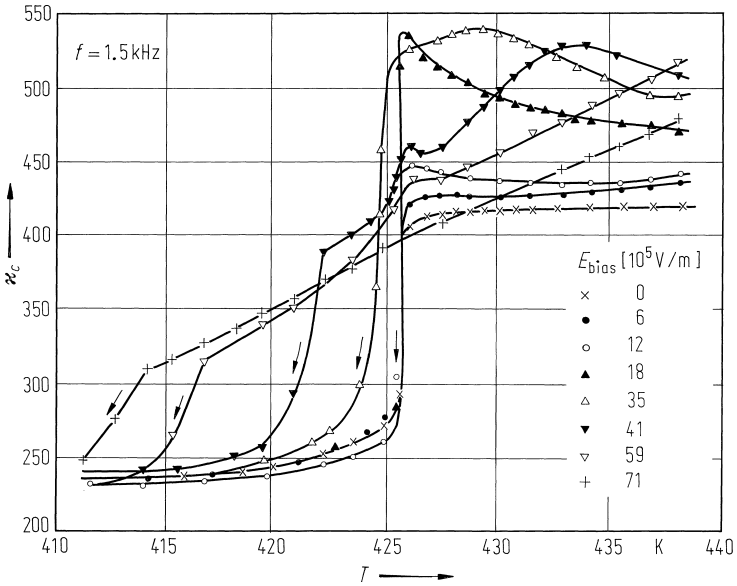

Fig. 1A-16-006. $PbHfO_3$. κ_c vs. T [86Bal]. Parameter: E_{bias}

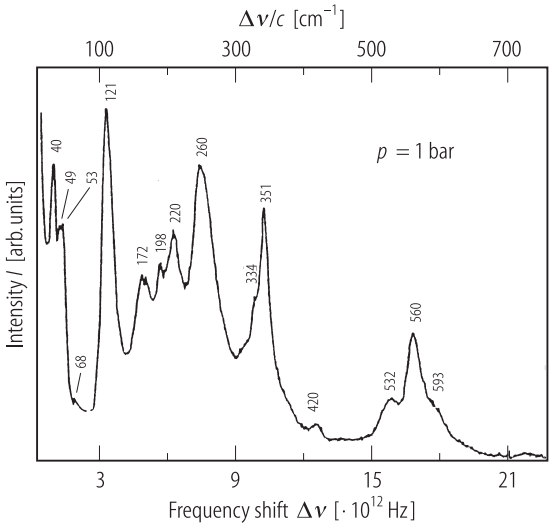

Fig. 1A-16-007. $PbHfO_3$. I vs. $\Delta\nu$ [94Jay].

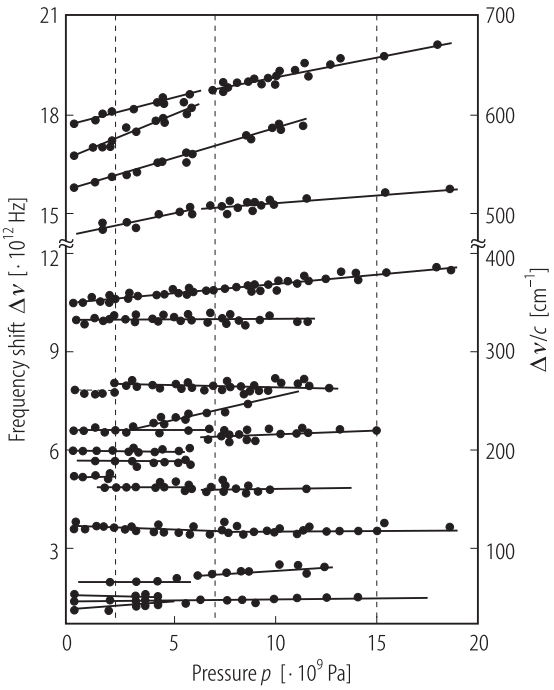

Fig. 1A-16-008. $PbHfO_3$. $\Delta\nu$ vs. p [94Jay].

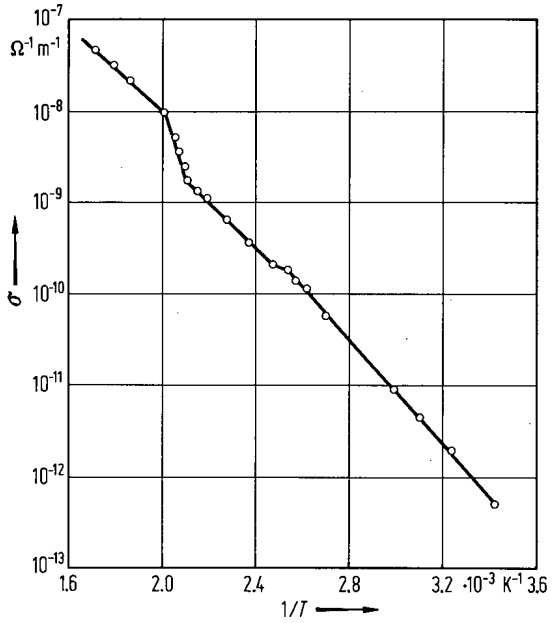

Fig. 1A-16-009. $PbHfO_3$ (ceramics). σ vs. $1/T$ [62Gur].

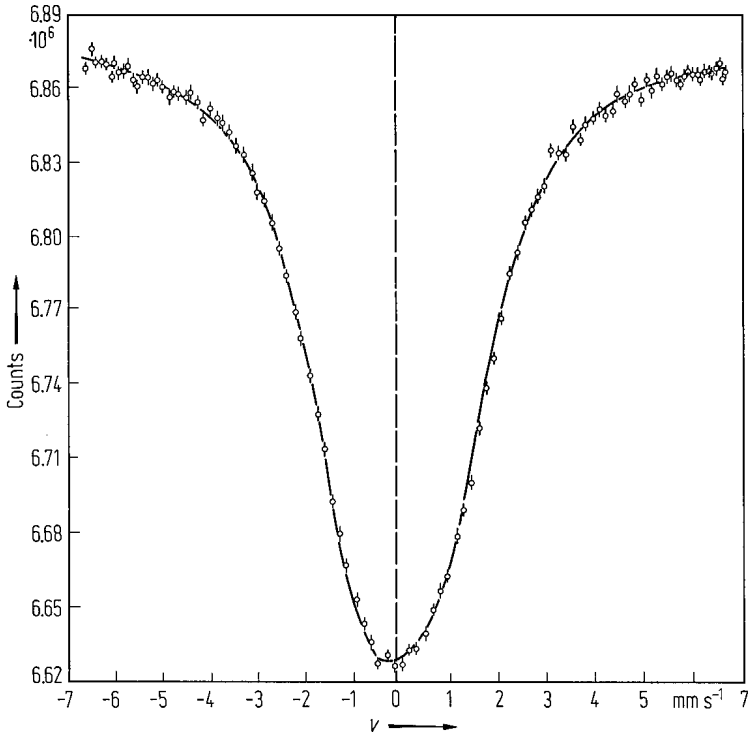

Fig. 1A-16-010. $PbHfO_3$. Mössbauer absorption spectrum [73For]. v: absorber velocity, ^{178}Hf as source.

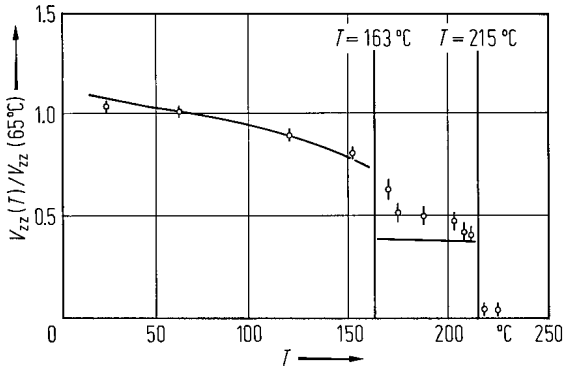

Fig. 1A-16-011. $PbHfO_3$. $V_{zz}(T)/V_{zz}$(65 °C) vs. T [73For]. V_{zz}: electric field gradient. The solid line represents the EFG calculated from the known lattice parameters by a lattice-sum calculation.

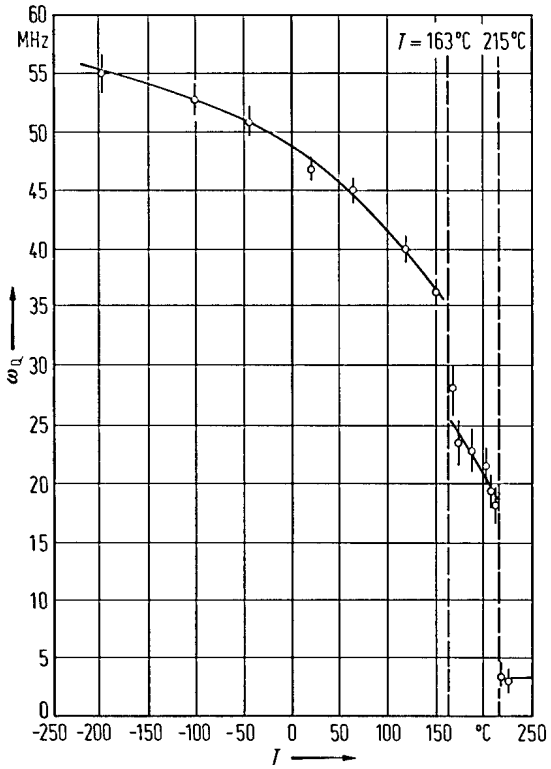

Fig. 1A-16-012. $PbHfO_3$. ω_Q vs. T [73For]. ω_Q: interaction frequency.

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