No. 20A-7 SbSI, Antimony sulfide iodide

(M = 280.71)

1a	Ferroelectricity in SbSI was discovered by Fatuzzo et al. in 1962. SbSI is the first example of ferroelectric substance showing large photoconductivity.			62Fat
b	phase	II	I	
	state	F [a])	P [a])	[a]) 62Fat
	crystal system	orthorhombic [c])	orthorhombic [b]) [c])	[b]) 50Don
	space group	$Pna2_1–C_{2v}^9$ [c])	$Pnam–D_{2h}^{16}$ [b]) [c])	[c]) 64Arn
	Θ [°C]	about 20, 22 [a]), 19 [d])		[d]) 64Mor
	P_s ∥ [001].			62Fat
	T_{melt} ≈ 400 °C.			64Mor
	ρ = 5.1(9) · 10^3 kg m^{-3} (observed), (ρ_X = 5.2 · 10^3 kg m^{-3}).			50Don
	Color: dark red, transparent at RT.			
	Cleavage: fibrous, along [001] direction.			60Nit
2a	Preparation: $SbI_3 + Sb_2S_3 \rightarrow 3SbSI$ (reaction in sealed, evacuated ampoule, 500 ... 600 °C).			60Nit
	Crystal growth:			
	Vapor transport, chemical transport method: see			62Ker, 67Kik, 71Nee
	Flux method: see			64Mor, 70Nas
	Zone melting: see			71Nee
	Bridgman-Stockbarger method: see			64Nit, 69Mas, 69Rob, 71Nee, 71Spi
	Hydrothermal method: see			69Rab, 69Pop, 70Pop1,
	High gas pressure synthesis: see			72Bok
	Phase diagram $SbI_3 – Sb_2S_3$: Fig. 20A-7-001.			
	See also			70Pop2
	Thin film growth by flash evaporation, source; SbSI powder. [a])			[a]) 85Sud
	See also			83Man, 83Gho, 82Luk
b	Crystal form: Fig. 20A-7-002.			
3a	Unit cell parameters:			
	a = 8.54 Å, b = 10.18 Å, c = 4.12 Å at 100 °C,			76Iwa
	a = 8.522(3) Å, b = 10.130(4) Å, c = 4.088(2) Å at 27 °C,			74Ito
	a = 8.51 Å, b = 10.02 Å, c = 4.12 Å at –185 °C.			76Iwa
	Additional data: Table 20A-7-001.			
	Temperature dependence of unit cell parameters: Fig. 20A-7-003.			

b	$Z = 4$ in phases I and II.	50Don
	Crystal structure: Table 22A-7-002; Fig. 20A-7-004, Fig. 20A-7-005.	
	Positional parameters at 1.3 °C, 27 °C and 48 °C: Table 20A-7-003, Table 20A-7-004.	
	For additional data at 5 °C and 35 °C, see	67Kik
	Interatomic distances in phases I and II: Table 20A-7-005, Table 20A-7-006, Table 20A-7-007; Fig. 20A-7-006, Fig. 20A-7-007.	
	Atomic shift in phase II relative to phase I, see	76Ito
	Neutron diffraction method, see	66Iwa, 76Iwa
	Temperature dependence of thermal vibrations and interatomic distances: Fig. 20A-7-008, Fig. 20A-7-009.	
	See also	74Ito
4a	Thermal expansion along the c axis: Fig. 20A-7-010, Fig. 20A-7-011.	
	Effects of light illumination on strain relaxation: Fig. 20A-7-012.	
	Linear compressibility along the c axis: Fig. 20A-7-013.	
5a	$\kappa_c = C/(T - \Theta_p)$, $T > \Theta_f$, where $C = 2.33 \cdot 10^5$ K, $\Theta_p = 16.0$ °C, Θ_f, = 19.2(2) °C;	64Mor
	see also	68Pik, 69Toy
	Dielectric constant at low frequency: Fig. 20A-7-014, Fig. 20A-7-015.	
	See also	78Iri, 74Iri
	Dielectric constant at microwave frequency: Fig. 20A-7-016, Fig. 20A-7-017.	
	Dielectric constant in a wide frequency range: see	71Bel
	Effect of laser light illumination on κ: see	71Bel
	Dielectric constant of thin films: Fig. 20A-7-018.	
	See also	73Yos, 83Man
	Dielectric constant of pressed powder, and particle size dependence: see	77Man
	Effect of hydrostatic pressure on κ: Fig. 20A-7-019.	
	Effect of hydrostatic pressure on Θ: Fig. 20A-7-020.	
	Additional information: see	75Sam, 65Gul, 68Sam, 68Ger, 69Ger
	For complex dielectric constants at microwave frequencies: see	83Gho, 79Bel
	Field induced shift of Θ_f: Fig. 20A-7-021.	
	Tricritical point at 235 K, $p \approx 1.4 \cdot 10^8$ Pa: see	78Sam
	Effect of uniaxial stress on Θ_f: Fig. 20A-7-022.	
	Bias field along the c axis: $d\Theta_f / dE = 2.66 \cdot 10^{-2}$ °C kV^{-1} m.	
	See also	69Toy, 68Pik
b	$\xi = -2.6 \cdot 10^8$ VC^{-3} m^5, $\zeta = 5.4 \cdot 10^9$ VC^{-5} m^9.	68Pik
	See also	68Kaw, 69Toy
c	Spontaneous polarization: Fig. 20A-7-023, Fig. 20A-7-024.	
	Effects of hydrostatic pressure: Fig. 20A-7-025.	
	Jump of P_s at Θ_f: $\Delta P_s \approx 18 \cdot 10^{-2}$ C m^{-2}.	68Kaw

	Data for polycrystalline sample: see	69Mas, 69Pan
	Spontaneous polarization and coercive field: Fig. 20A-7-026.	
d	Effects of poling and of light illumination upon the pyroelectric effect: see	66Ima, 68Mih
	Pyroelectric detector sensitivity, ≈ $2.6 \cdot 10^{-3}$ C m^{-2} K^{-1} at 300 K.	70Pan
	Pyroelectric coefficient: Fig. 20A-7-027.	
6a	Heat capacity: Fig. 20A-7-028, Fig. 20A-7-029.	
	See also	72Tar
	Additional data, transition heat and transition entropy: see	65Mor, 68Pik, 72Tar
b	Termal conductivity along the *c* axis: Fig. 20A-7-030.	
7a	Piezoelectric constant d_{33}: Fig. 20A-7-031.	
	See also	64Ber, 72Ham, 72Sch
	Electromechanical coupling constant k_{33}: Fig. 20A-7-032.	
	See also	64Ber
	Mechanical and piezoelectrical properties of crystals precipitated with a special treatment: see	86Yon
b	Electrostrictive constant Q_{33}: Fig. 20A-7-033.	
	See also	72Sch
	$\lvert Q_{13} \rvert < 10^{-2}$ m^4 C^{-2}, $Q_{23} = -0.05$ m^4 C^{-2}, $Q_{33} = 0.19$ m^4 C^{-2}.	72Ham
8a	Elastic compliance and stiffness: Table 20A-7-008; Fig. 20A-7-034.	
	see also	64Ber, 72Ham
	Sound velocity and attenuation at 10 MHz: Fig. 20A-7-035.	
	Sound velocity and attenuation under a dc bias field: Fig. 20A-7-036, Fig. 20A-7-037.	
	For additional information, see	70Zap, 75Zap, 70Bel
	Microhardness of an ingot crystal at RT: see	86Pal
b	Second acoustic harmonic generation and Grüneisen coefficient: see	71Sam
9a	SbSI is negative biaxial. Optic angle $2V$ (the acute angle between the optic axes) is approximately 83°: see	67Joh
	Refractive index at $\lambda = 633$ nm: $n_a = 2.87$, $n_b = 3.63$, $n_c = 4.55$ at 22 °C; $n_a = 2.87$, $n_b = 3.57$, $n_c = 4.44$ at 12 °C: see	70San
	Refractive indices:	
	Dependence on λ: Fig. 20A-7-038, Fig. 20A-7-039.	
	Temperature dependence: Fig. 20A-7-040, Fig. 20A-7-041, Fig. 20A-7-042.	
	Effects of dc bias field: Fig. 20A-7-043, Fig. 20A-7-044.	
	Reflectivity spectra, and dielectric constant obtained in terms of the Kramers-Kronig relation: Fig. 20A-7-045, Fig. 20A-7-046, Fig. 20A-7-047, Fig. 20A-7-048, Fig. 20A-7-049, Fig. 20A-7-050.	
	See also	69Pet, 70Sug, 70Pet, 71Agr

	Absorption and transmission: Fig. 20A-7-051, Fig. 20A-7-052, Fig. 20A-7-053, Fig. 20A-7-054, Fig. 20A-7-055. Ferroelectric soft mode frequency: Fig. 20A-7-056. See also band gap E_G data in subsection 11 below. Electroreflectance, see subsection 11 below.	
b	Electrooptic constant: see	70Ohi
e	Quadratic electrooptic constant: see	77Mam
	Second harmonic generation: information on the optical nonlinear susceptibilities and effects of electric field: see	70Haf
10a	Raman scattering: Intensity vs. frequency: Fig. 20A-7-057, Fig. 20A-7-058. Effects of pressure: Fig. 20A-7-059, Fig. 20A-7-060, Fig. 20A-7-061, Fig. 20A-7-062. See also	70Har, 70Chi, 70Per, 71Agr, 71Ste, 81Bru, 82Afa
b	Brillouin scattering: Table 20A-7-008; see also	70San
11	Conductivity: Fig. 20A-7-063. See also	86Pal, 83Man
	Conductivity under a dc bias field: Fig. 20A-7-064.	
	Conductivity σ_{dark} of as grown crystal at RT is usually of the order of 10^{-6} Ω^{-1} m^{-1} along the *c* axis; see also	64Sas 65Saw, 71Kat, 69Neu, 72Art, 75Ado
	Increase of dark conductivity ρ by X-ray irradiation: see	81Eis
	Dark current measurements: $\rho \approx 3.107$ Ωm at RT.	
	Activation energy: $E \approx 0.59(1)$ eV, $T > \Theta_f$ (dark current ∝ exp (– E/kT)).	80Cha
	Band gap: Fig. 20A-7-065. See also	84Iba, 86Gra
	Electronic band structure: Fig. 20A-7-066. See also	84Zic
	Activation energy and information on trapping center, see	66Nos, 66Ale, 73Iri
	Photoconductivity at RT shows a maximum at about $\lambda = 600$ nm.	60Nit, 66Hav, 73Fri, 70Bez, 70Fri, 71Nes
	Photoluminescence: see	75Aga
	Temperature dependence of absorption edge: Fig. 20A-7-067. See also subsection 9 above.	
	Amount of shift ΔE_G of the absorption edge depends on P_s.	72Ish

	$\Delta E_G = \beta P_s^2 + \gamma P_s^4$ with $\beta = 1.38$ eV m^4 C^{-2}, $\gamma = -7.23$ eV m^8 C^{-4}.	
	Effect of E_{bias} on the absorption edge: Fig. 20A-7-068, Fig. 20A-7-069.	
	See also	63Har
	Effect of hydrostatic pressure on the absorption edge: Fig. 20A-7-070.	
	Life time of photo-excited charge carriers: see	66Nos
	Excitation of trapped carriers, thermally stimulated current behavior: see	70Toy, 73Iri
	Piezoresistance: see	70Zav
	Thermoelectric power: Fig. 20A-7-071.	
	Electroreflectance $\Delta R/R$: Fig. 20A-7-072.	
	See also	78Zam
	Electronic band structure: Fig. 20A-7-073, Fig. 20A-7-074.	
	For the band structure and the density of state: see also	71Nik, 74Fon
12	Magnetic susceptibility: Fig. 20A-7-075; see also Fig. 20A-1-004 in No. 20A-1.	
	Raman scattering under strong magnetic field: see	81Bru
13a	NMR and NQR: Table 20A-3-005; Fig. 20A-7-076.	
	See also	66Kra, 69Kra, 70Pop3, 72Kra
	NQR of ^{121}Sb: Fig. 20A-7-077.	
c	Mössbauer effect: Fig. 20A-7-078; see also Table 20A-3-006 in No. 20A-3.	
	See also	72Ale, 75Don, 73Tum
14	Diffraction phenomena: Fig. 20A-7-079.	
	For diffuse X-ray scattering, see	77Low
	Inelastic neutron scattering: Fig. 20A-7-080, Fig. 20A-7-081.	
15	Domains: see	70Kli1, 70Kli2, 71Ben
	Domain switching: Fig. 20A-7-082; see also	69Bog, 69Kud, 69Rud
	Characteristic patterns observed with a microscope: Fig. 20A-7-083, Fig. 20A-7-084.	
	See also	62Ker, 69Tra
16	Dilatation caused by photoillumination: Fig. 20A-7-012.	
	See also	70Gre
	Acoustoelectric effect for ultrasonic waves: see	69Kun
	Thin film and surface layer: see	70Mck, 72Ham, 78Bez
	Optical bistability due to photoinduced carriers: see	81Uch