

substance: PtSb₂**property: electronic properties**

The valence band maxima are six ellipsoids on [100] axes, with $K = m_{\parallel}/m_{\perp} = 0.87$ (low T)...0.67 (high T). The eight conduction band minima lie on [111] axes, with $m_{\parallel}/m_{\perp} = 1.43$ (low T)...1.36 (high T). Both the valence and conduction bands are derived from Pt d-orbitals with an additional higher-energy s-like conduction band [65E, 72D, 83D].

energy gaps

$E_{g,th}$	≥ 0.05 eV		from $\log \rho \propto E_g/2kT$	63H
			polycrystalline sample	
	0.06 eV		from $\rho(T)$ and $R_H(T)$,	65J
	0.075 eV	$T = 0$ K	single crystal and polycrystal	
			from $\log \rho \approx 0.4 E_g/kT$,	65D
			assuming $(\mu_n + \mu_p)(p \cdot n)^{1/2}$	
	0.11 eV		temperature independent	
			from resistivity, Hall effect	73A
			and Nernst-Ettingshausen effect	
			on single crystals	
	0.112 eV		from $\log \rho \propto E_g/2kT$ in the intrinsic	68E
			region, $T = 120...300$ K,	
			single crystals	
	(0.110 – 0.00015T) eV		from resistivity and Hall effect on	83D
			Te doped single crystals;	
			ac method,	
			100Hz, frequency independent	
			50...10 ⁴ Hz, T in K	
$E_{g,ind}$	≈ 0.10 eV		indirect gap from optical	65D,
			absorption	68R,
				70O,
				72D
	0.104...0.113 eV	$T = 10$ K	band-to-band indirect absorption	68R,
			threshold	70O
$E_{g,dir}$	> 0.4 eV	$T = 4$ K	from the energy dependence of the	72D
			cyclotron mass	
			$m_{\omega_c}(E) = m_{\omega_c}(0)/(1+(2E/E_{g,dir}))$;	
			m_{ω_c} changes by less than 5%	
			when E increases by 0.11 eV	

donor levels

E_d	2.3 eV		ionization energy of an isolated	76A
			donor (Te doped sample)	
	3...4 eV		from $\rho(T)$ of Te-doped samples	68R
	3...5.5 eV			83D

effective masses

$m_{n,p} = n_{C,V}^{2/3}(m_1 m_2 m_3)^{1/3} = n_{C,V}^{2/3} m_{||}^{1/3} m_{\perp}^{2/3} = n_{C,V}^{2/3} (m_N)_{C,V}$; n_C , n_V are the numbers of ellipsoids in conduction and valence band, respectively

$m_{n }$	0.53...0.66 m_0	low T ...high T	calculated from theoretical band model based on experimental data from [65D]	65E
$m_{n\perp}$	0.37...0.49 m_0	low T ...high T		
$(m_N)_C$	0.42...0.54 m_0	low T ...high T	density of states effective mass	65E
	0.5 m_0	low T		65D
m_n^c	1.6 m_0	$T = 360$ K	conductivity effective mass of a single ellipsoid	73A
			$3(m_1^{-1} + m_2^{-1} + m_3^{-1})^{-1}$ derived from the edge of the plasma reflection	
	0.35 m_0	$T = 50$...100 K	conductivity effective mass for a single valley in the conduction band	83D
	0.34...0.57 m_0	$T = 77$ K	conductivity effective mass, from optical absorption, assuming acoustic-phonon scattering or ionized-impurity scattering (upper limit)	68R
$m_{p }$	0.52...0.55 m_0	low T ...high T	based on theoretical band model and data from [65D]	65E
	0.35 m_0	$T = 77$ K	using the theoretical model of [65E] with $m_{ }/m_{\perp} = 0.77$	73A
	0.66 m_0	$T = 310$ K		
$m_{p\perp}$	0.60...0.82 m_0	low T ...high T		65E
	0.45 m_0	$T = 77$ K		73A
	0.85 m_0	$T = 310$ K		
$(m_N)_V$	0.57...0.72 m_0	low T ...high T	density of states mass of a single ellipsoid	65E
	0.22 m_0	$T = 4$ K		65D, 72D
	0.41 m_0	$T = 77$ K	from $S(T)$ assuming acoustic-phonon scattering only ($m_p = 1.34 m_0$)	73A
	0.17...0.30 m_0	$T = 77$ K	conductivity effective mass, from	68R
	0.2 m_0	$T = 300$ K	optical absorption from plasma reflection	83D
	1.0 m_0	$T = 360$ K	conductivity effective mass from	73A
			the edge of the plasma reflection	
	0.168 m_0	$T = 1.3$...4.4 K $B < 6$ T	least cyclotron mass $(m_1 m_2)^{1/2}$ from high-field magnetoresistance on p-type single crystals	72D

anisotropy of valence band principal effective masses: $m_1:m_2:m_3 = 0.61:1:1.64$ ($= 0.134:0.22:0.361$) from Shubnikov-de Haas oscillations [72D]. Group-theoretical arguments, however, require that in space group Pa3 of the pyrite structure the [100] ellipsoids should have two equal principal masses [83D].

For the temperature dependence of the density-of-states mass, see Fig. 1.

References:

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Fig. 1.

PtSb₂. Density of states effective masses of electrons and holes vs. temperature in a doubly-logarithmic scale [73A].

