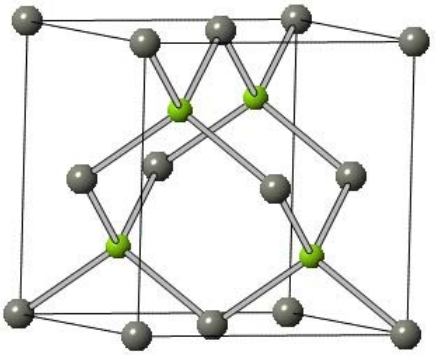
Search

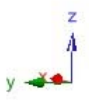
Material: Zinc Selenide (ZnSe)

Basic Info

ZnSe is a light yellow binary solid compound that is rarely occurs in nature. It can be made in hexagonal and cubic crystal structures. Zinc selenide is used as a blue light source in light-emitting diodes and diode lasers. It is also used as infrared laser gain medium and as an infrared optical material. ZnSe activated with tellurium is used in x-ray and gamma ray detectors as a scintillator. [9]

Crystal Structure





			Fractional Coordinates			Orthogonal Coordinates		
	Label	Elmt	x	y	z	xor[Å]	yor[Å]	zor[Å]
1.	T2	Se	0.2500	0.2500	0.2500	-0.863	-1.331	-1.873
2.	T2	Se	0.2500	0.7500	0.7500	0.100	-3.980	-4.722
3.	T2	Se	0.7500	0.7500	0.2500	-2.657	-1.164	-5.453
4.	T2	Se	0.7500	0.2500	0.7500	-3.482	-4.171	-2.935
5.	T1	Zn	0.0000	0.0000	0.0000	0.000	0.000	-0.000
6.	T1	Zn	0.0000	0.5000	0.5000	0.963	-2.649	-2.849
7.	T1	Zn	0.5000	0.5000	0.0000	-1.794	0.167	-3.580
8.	T1	Zn	0.5000	0.0000	0.5000	-2.620	-2.841	-1.063
9.	T1	Zn	1.0000	0.0000	0.0000	-5.376	-0.025	-1.793
10.	T1	Zn	1.0000	0.5000	0.5000	-4.414	-2.674	-4.642
11.	T1	Zn	0.0000	1.0000	0.0000	1.788	0.358	-5.366
12.	T1	Zn	0.5000	1.0000	0.5000	-0.831	-2.482	-6.429
13.	T1	Zn	1.0000	1.0000	0.0000	-3.588	0.333	-7.159
14.	T1	Zn	0.0000	0.0000	1.0000	0.137	-5.656	-0.332
15.	T1	Zn	0.5000	0.5000	1.0000	-1.657	-5.490	-3.912
16.	T1	Zn	1.0000	0.0000	1.0000	-5.239	-5.681	-2.125
17.	T1	Zn	0.0000	1.0000	1.0000	1.925	-5.298	-5.698
18.	T1	Zn	1.0000	1.0000	1.0000	-3.451	-5.323	-7.491

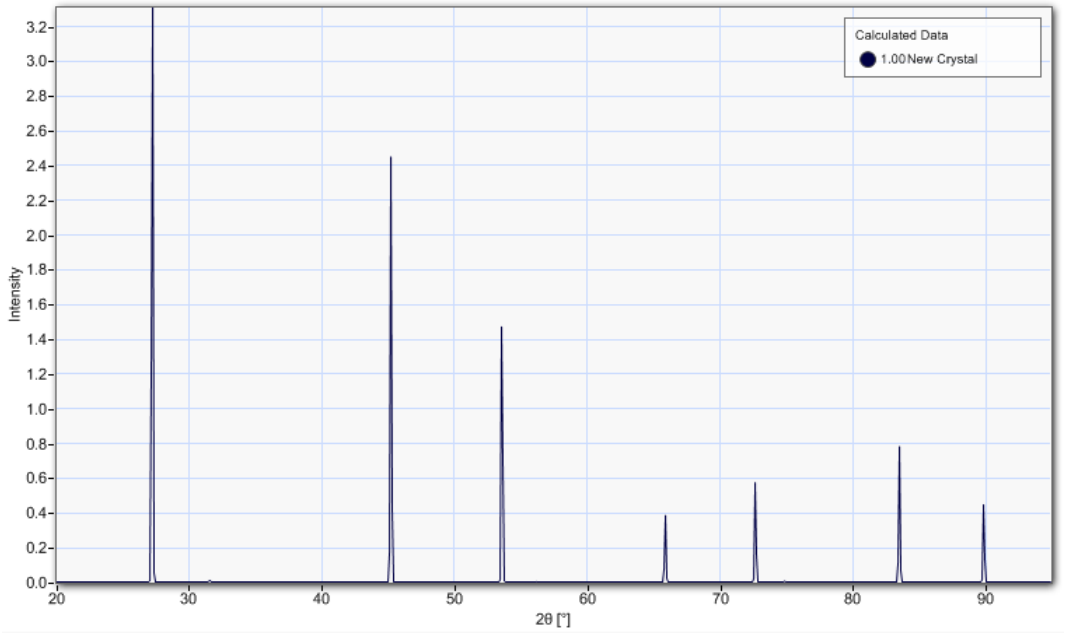
Theoretical diffraction data using a Cu Kα monochromatic source.

(m is the multiplicity and N is the maximum number of flexions)

ref no.	h	k	l	d(hkl)	2-Theta	Intensity	I/Imax	m	N
[1]	1	1	1	3.27219	27.2296	3.56799e-001	100.0	8	3
[2]	0	0	2	2.83380	31.5438	1.03393e-003	0.3	6	4
[3]	0	2	2	2.00380	45.2123	2.62259e-001	73.5	12	8
[4]	1	1	3	1.70885	53.5827	1.57080e-001	44.0	24	11

[+] Feedback

[5]	2	2	2	1.63610	56.1706	3.14514e-004	0.1	8	12
[6]	0	0	4	1.41690	65.8603	4.10933e-002	11.5	6	16
[7]	1	3	3	1.30024	72.6539	6.12994e-002	17.2	24	19
[8]	0	2	4	1.26731	74.8585	6.43795e-004	0.2	24	20
[9]	2	2	4	1.15689	83.4861	8.34838e-002	23.4	24	24
[10]	1	1	5	1.09073	89.8496	4.77530e-002	13.4	32	27
[11]	0	4	4	1.00190	100.4906	3.01446e-002	8.4	12	32



PV Applications

ZnSe thin films are prepared primarily by molecular beam epitaxy, chemical vapor deposition, chemical vapor deposition, and vacuum evaporation. Electrodeposition is a simple, low cost and a viable method for producing good quality films.[2]

ZeSe films prepared by chemical vapor deposition have a buffer layer that has reached total area efficiencies of up to 9.6% (under AM 1.5 illumination), an open circuit voltage of 482 mV, a short circuit current of 31.0 mA/cm^2 and a fill factor reaching 64%. [8]

Basic Parameters at 300 K

Crystal structure:	Sphalerite	[1]
Group of symmetry:	F−43m	[1]
Number of atoms in 1 cm^3:	4.39*10^{26}	[1]
Unit cell volume:	182.05 Å^3	[1]
Atoms per unit cell:	8	[1]
Debye temperature:	339(2) K	[7]
Density:	5.266 g/cm^3	[1]
Dielectric constant (static):	8.6	[10]
Dielectric constant (high frequency):	5.7	[10]
Effective electron masses:	(0.16 ± 0.01)m$_e$	[3]
Effective hole masses:	0.75 m$_o$	[7]
Lattice constant:	a = 5.667 Å	[1]
Optical phonon energy (longitudinal):	0.0314 eV	[5]
Conductivity:	n−type	[3]

Temperature Dependences

Graph of electron concentration vs temperature may be found in M. Aven, High Electron Mobility in Zinc Selenide Through Low Temperature Annealing. J. Appl. Phys. 42, 1204 (1971); doi: 10.1063/1.1660167 [5]

Donors and Acceptors

Donors:	Al, Cl, Ga, In, F, Br	[3],[4]
Acceptors:	Cu, Ag, Sb	[4]

Ionization energy of shallow donors [7]

$E_d(Li_I)$	15(1) meV	T= 4.2 K
$E_d(Na_I)$	16(1) meV	

E_d(Al)	26.3 meV
E_d(Ga)	27 meV
E_d(In)	28.1 meV
E_d(F)	29.3 meV
E_d(Cl)	26.1 meV
E_d(I)	30.4 meV

Ionization evergy of shallow acceptors

E_a(Li)	118(2) meV T = 4.2 K
E_a(Na)	98(2) meV
E_a(K)	94(2) meV
E_a(N)	112 meV T = 4.2 K
E_a(P)	80...92 meV T = 4.2 K
E_a(As)	125 meV T = 77 K
E_a(Sb)	69 meV T = 30 K
E_a(Rb)	89(2) meV T = 4.2 K
E_a(Cs)	74(2) meV
E_a(O)	80 meV T = 4 K
E_a(V_{Zn})	218 meV T = 4 K

Electrical Properties

Basic Parameters of Electrical Properties

Energy gap: 2.81 eV [2]

Energy spin-orbital splitting:	Δ_0 (Γ_{8v}- Γ_{7v})	0.42 eV	T=295 K	[7]
	Δ_1 ($\Gamma_{4,5v}$- Γ_{6v})	0.20 eV	T=300 K	[7]

Donor concentration: 10^{16} cm^{-3} [5]

Carrier mobility:	μ_n = up to 400 cm^2/Vs	T=300K	[7]
	μ_p = 110 cm^2/Vs	T=300K	[7]

Intrinsic resistivity: ~10^{12} Ω cm [6]

Mobility and Hall Effect

Hall mobility:	530 cm^2/ V*s (T=300 K)	[6]
	12,000 cm^2/ V*s (T=60 K)	[6]
Absorption coefficient:	10^4 cm^{-1}	[2]

Mobilities and mobility ratios as well as a graph of electron hall mobility vs temperature may be found in:

M. Aven, High Electron Mobility in Zinc Selenide Through Low Temperature Annealing. J. Appl. Phys. 42, 1204 (1971); doi: 10.1063/1.1660167 [5]

Optical properties

Refractive index: Graph of refractive index and absorption index vs. photon energy may be found in Madelung, O. (2004). *Semiconductors: Data handbook*. (3rd ed., pp. 736-757). Springer. [7]

Thermal properties

Coefficient of linear thermal expansion:	$\alpha = 7.4*10^{-6}\ K^{-1}$	[7]
Heat capacity:	$C_p = 51.88$ J/Mol*K	[7]
Thermal conductivity	$\kappa = 0.19\ W\ K^{-1}\ cm^{-1}$ T=300K	[7]

Graphs of ZnSe's thermal properties may be found in Madelung, O. (2004). *Semiconductors: Data handbook*. (3rd ed., pp. 736-757). Springer. [7]

Mechanical properties, elastic constants, lattice vibrations

Basic Parameters

Bulk modulus:	62.4(7) GPa	[7]
Density:	5.266 g/cm^3	[7]

Elastic Constants

Elastic Constants:	$C_{11} = 90.3(19)$ GPa	[7]
	$C_{12} = 53.6(23)$ Gpa	[7]
	$C_{44} = 39.4(12)$ Gpa	[7]

Phonon Frequencies

$V_{LO}(\Gamma)$	7.59 THz	T=300 K	[7]
$V_{TO}(\Gamma)$	6.39 THz	T=300 K	

Phonon Energies

$Hv_{LO}(\Gamma_1)$	30.99 meV [7]
$Hv_{TO}(\Gamma_{15})$	25.17 meV
$Hv_{LA}(\Gamma)$	19.8 meV
$Hv_{TA}(\Gamma)$	8.0 meV
$Hv_{LO}(X)$	27.64 meV
Hv_{TO}	25.54 meV
Hv_{LA}	23.55 meV
$Hv_{LO}(L)$	27.77 meV
Hv_{TO}	25.54 meV
$Hv(W_3)$	24.9 meV
$Hv(W_1)$	18.59 meV
$Hv(W'_2)$	11.53 meV
$Hv(W''_2)$	26.53. meV
$Hv(W'_4)$	14.26 meV
$Hv(W''_4)$	24.61 meV

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‹ SnS CuInSe2 ›

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