Study of Zinc Blende and Wurtzite Zns

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Abstract:
ZnS has a unique structure type compared to other molecules, having different types of unique structures. ZnS Structural Information and ZnS can have a zinc blende structure which is a "diamond-type network" and at a different temperature, ZnS can become the wurtzite structure type which has a hexagonal type symmetry. Structure-wise, the zinc blende structure is more thermodynamically favored, however, because of the wurtzite structures slow construction, both forms of ZnS can be found.

Summary
Zinc blend is a compound that comes in two forms: sphalerite and wurtzite. These are characterized by a 1:1 stoichiometric ratio of Zinc to Sulfur. It maintains a tetrahedral arrangement in both forms. ZnS Structural Information

1. Introduction

Zinc sulfide (ZnS) is a unique compound that forms two types of crystalline structures.[1] These two polymorphs are wurtzite and zincblende (also known as sphalerite).[3]Wurtzite has a hexagonal structure, while zincblende is cubic.[1] It is characterized by single bonds between each atom and maintenance of a 1:1 zinc to sulfur ratio.[4] ZnS is the most important base material for cathode-ray tube luminescent materials. In order to meet the requirements of various types of luminescent screen, routes to ZnS powder with adjustable particle morphology were investigated. The most important morphological. Application of precipitated ZnS as a phosphor raw material requires conservation of shape during the heat treatment necessary (typically 900—1000 °C). Upon firing at this temperature, the grain is densified first and loses its internal structure.

2. Sphalerite

Site	Zn	S
Central	4	0
Face	0	6(1/2)=3
Corner	0	8(1/8)=1
Total	4	4

Since the number of atoms in a single unit cell of Zn and S is the same, it is consistent with the formula ZnS.The ionic radius for Zn^{2+} is 74pm and for S^{2-} is 190pm. Therefore the ratio between cationic and anionic radii in zinc blend is 0.39 (74pm/190 pm) .This suggests a tetrahedral ion arrangement and four nearest neighbors from standard crystal structure prediction tables. Therefore, four sulfur atoms surround each zinc atom and four zinc atoms surround each sulfur atom.$_2$ The coordination number, the number of of electron pairs donated to a metal by its ligands, for both zinc an sulfur is four.[1,2] The difference between wurtzite and zincblende lies in the different arrangements of layers of ions.[2]

3. Structural Information

Zincblende Vital Statistics	
Formula	Zns
Crystal System	Cubic
Lattice Type	Face-Centered
Space Group	F4(bar)3m,no..??
Cell Parameters	a=5.41Å ,Z=4
Atomic Positions	S-0,0,0 Zn-0.25,0.25,0.25 (can interchange if desired)
Density	4.102
Melting Point	Phase transition at 1020 degrees C
Alternate Name	Zincblende,sphalerite
Isostructural Compounds	$AgInS_2$, BN,BC.XY(X=Al,Ga,In,Y=P,As,Sb)

4. Zincblende (Sphalerite)

Zincblende is characterized as a cubic closet packing (ccp), also known as face-centered cubic, structure.[1,4] This crystal lattice structure is shown in Figures 1 & 2 below. The discussion of corresponding zincblende and wurtzite states is helpful in understanding the nature of the energy states in mixed crystals: (wurtzite structure [111] twinned on zincblende), and in faulted crystals: [111] stacking faults.

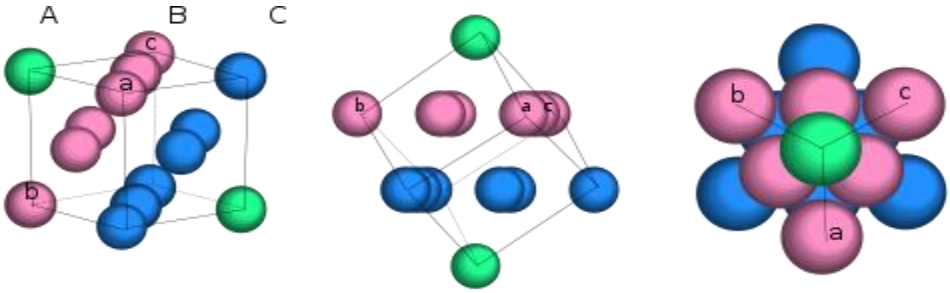

Fig. 1. A break down of cubic closest packing.

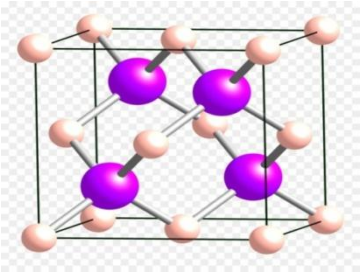

Fig. 2. A representation of ccp structure. (from Public Domain)

5. Thermal stability

Density tends to decrease as temperature increases. In this case, since ccp structures are more dense than hcp structures, so a conversion from sphalerite to wurtzite occurs naturally over time at a rate similar to that of diamond to graphite. The sphalerite structure is favored at 298k by 13kJ/mol, but at 1296K the transition to wurtzite occurs.[3]

6. Wurtzite

Wurtzite has a hexagonal closest packing structure (hcp), which is characterized by 12 ions in the corners of each unit that create a hexagonal prism (seen in Fig. 3).[2] As discussed previously, zincblende slowly transforms to wurtzite due to thermodynamic stability.

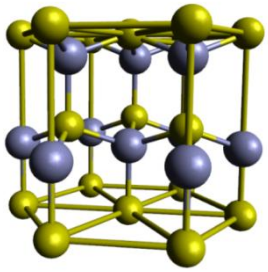

Fig 3. HCP structure of wurtzite.

Calculating density of a crystal structure:
Density = Mass of unit cell / volume of unit cell.
where:
Mass of unit cell = Number of atoms in a unit cell x the mass of each atom
volume of unit cell = $a^3 \times 10^{-30}$

7. Conclusions

The ZnS nanoparticles were successfully synthesized through chemical co-precipitation method and X-ray diffraction was employed to study the structural properties, the particle sizes calculated were have zinc blended structure.The ZnS nanoparticles of manganese doped zinc sulfide have been successfully synthesized by a simple precipitation reactionusing aqueous in which mercaptoethanol was used as a capping agent. In this work we prepared ZnS thin films by chemical bath deposition (CBD). The ZnS thin film deposition process clearly shows three different growth phases. The XRD pattern of the as-deposited and annealed ZnS film exhibited peaks corresponding to the (1 1 1), (2 2 0), (3 1 1) plane of the cubic ZnS.

Reference

1. Shen, G. Z. Y. Bando, J. Q. Hu, and D. Golberg, Appl. Phys. Lett. 90, 123101 (2007).
2. Cyr, P.W. M. Tzolov, M.A. Hines, I. Manners, E.H. Sargent, G.D. Schools, Quantum dots in a metallopolymer host: studies of composites of polyferrocenes and CdSe nanocrystals, J. Mater.Chem..
3. Devi, B S Rema R Raveendran and A V Vaidyan Pramana, 2007, 68, 4 679
4. Bloss, W.H., F. Pfisterer, H.W. Schock, "Advances in Solar Energy, An annual review of research and Development.
5. Ubale, A.U. and D.K. Kulkarni, 2005. Bull. Mater. Sci. 28(1) 42-47