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Properties of Zinc Oxide

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Abstract
In this paper, we studied about Properties of Zinc Oxide.

Keywords
Zinc Oxide, Tetrahedral symmetry.

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Contents

1. Crystal structure of Z_nO

General, Zinc oxide crystallizes in two main forms, hexagonal wurtzite and cubic zinc blende but the (B4 type) wurtzite structure is obtained only at optimum pressure and temperature[23,28]. In an ideal wurtzite crystal, with a hexagonal close-packed lattice type, has lattice parameters, ao= 0.32495 nm and co = 0.52069 nm, in the ratio of co / ao =1.602, and it belongs to the space group of P63mc[23,27] and is characterized by two interconnecting sub lattices of zn2+ and o2- where each anion is surrounded by four cations at the corners of a tetrahedron with a typical sp3 covalent bonding. Among different phases of ZnO, based on the first principle periodic Hartree-Fock linear combination of atomic orbitals theory the wurtzite is found to be the most thermodynamically stable phase[23].

Tetrahedral symmetry plays a vital role for the polarity of ZnO that arises along the hexagonal axis. Piezoelectricity and spontaneous polarization are the direct consequence of polar symmetry of ZnO along the hexagonal axis[23]. The structure of ZnO, can be described as a number of alternating planes composed of tetrahedrally coordinated O2- and Zn2+ ions, stacked alternately along the C-axis (Figure.2.1.)The oppositely charged ions produce positively charged(0001)-Zn and negatively charged (0001)-O polar surfaces, resulting in a normal dipole moment and spontaneous polarization along the c-axis, as well as a divergence in surface energy [25-26].The polar faces are more stable than non polar faces.

The root cause for the natural N-type nature of ZnO is due to the sensitiveness of ZnO lattice constants to the presence of structural point defects (vacancies and interstitials) and extended defects (threading/planar dislocations) that are commonly found in ZnO resulting in a non-stoichiometric compound Zn1+d O with an excess zinc .These excess zinc atoms have the tendency to function as donor interstitials that give its natural N-type conductivity. In ionic form, the excess zinc exist as Zn+ interstitials that are mobile and they tend to occupy special interstitial sites with Miller index (1/3, 2/3, 0.875)

These special sites offer passage routes for zinc interstitials to easily migrate within the ZnO wurtzite structure[36]. ZnO unit cell with ionic positions of zinc and oxygen atoms. Redrawn from [47]. Zinc interstitial sites in the ZnO wurtzite lattice.

2. Optoelectronic Property

The most important factor responsible for a material to show a better optoelectronic property is the large exciton binding energy and this property is posseessed by Zinc oxide having binding energy of 60mev which could be attended at and above room temperature due to excitonic recombination[29]. The process of optical absorption and emission have been influenced by bound excitons which are extrinsic transition related to dopants or defects thereby usually responsible for creating discrete electronic states in the band gap.

Theorytically,neutral or charged donors and acceptors are the members by which exciton could be bound with and it merely depends on the band structure of semiconductor material[29,30]. Thus exciton which is a bound system it do not requires traps to localize carriers and recombines with high efficiency.The piezoelectrically induce field makes deeper exciton of ZnO more stable against field ionization. Magnesium

doped zinc oxide possesses a wide range of sensing spectra between (200-280)nm which makes it suitable to tune for UV-B and UV-C and can be made applicable for various fields such as solar UV radiation monitoring,ultrahightemperature flame detection etc[24].

Zinc oxide films made from single crystal shows directionally dependent optical properties due to which it can be applied for modulation of UV radiation. The current example of it is the designed model of ZnO modulator with a contrast of 70:1 and operation speed of 100ps [24]. Also high breakdown stress and high saturation velocity of zinc oxide increases its demand for the different electronic application.PL spectra of ZnO nanowire shows increase of green emission intensity with a decrease of nanowire diameter and continuous reduction of diameter of ZnO nanowire gives quantum size effect and due to this size confinement exciton binding energy is enhanced. Transport characteristics and interaction of phonon with free carrier have impact on the performance of optoelectronic devices which can be acquired by the knowledge of vibrational properties of the material. The excellent emitting power of ZnO has been investigated through different reports and line width of excitonic recombination is as narrow as 40 μeV with fine spectroscopic details have been observed. The refractive index of wurtzite ZnO as reported [23,27] is nw = 2.008 and ne = 2.029[36]

3. Optical band gap

As reported from various literatures the band gap of ZnO films mostly depends on the carrier concentration and is found to be 3.37ev on basis of carrier concentration of 1018 -1020/cm3. Anamolous change (increase) in band gap has been observed when the carrier concentration is 5 $\times$ 1018/cm3 , and then a sudden decline in band gap [23,24],when concentration changes to 3-4 $\times$ 1019/cm3. .Quantum confinement of electrons in small grains created by potential barriers at the grain boundaries are thought to responsible for the drastic change in band gap. Sometimes also at higher doping concentration on a blue shift towards shorter wavelength has been observed and can be explained on the basis of Burstein–Moss effect[30,31].According to which increase of the carrier concentration due to Al doping results in a shift of the Fermi level and block some of the lowest states, thereby causing widening of the band gap resulting in the blue-shift of the absorption tail. The band gap of ZnO as calculated by local density approximation (LDA) is found to be 3.77ev which mostly accounts for the Zn 3d electrons [23,24] as shown in the figure.2.4. The ZnO having direct band gap is very well indicated by the valence band maxima and lowest conduction band minima both occurring at the same Γ point of k=0.Zn 3d levels are indicated by bottom ten bands (occurring around 9ev) and O 2p bonding states are highlighted by next six bands from -5eV to 0eV. The empty Zn 3s levels signified by first two conduction band states are mainly Zn localized. Crystallization of ZnO mostly favourable in wurtzite symmetry and crystal field splitting as well as spin orbit interaction results in three states say A, B &C figure.2.4.The symmetry of the A valence sub band is considered to be Γ7 based on the polarization properties of the free exciton transitions where as contradicting to it the most recent magneto-optical studies of the free exciton transition fine structure interpreted the symmetry to be Γ9. But the controversy is continuing as before 40 years ago.

4. Application of Z_nO nanostructures

Zinc oxide due to its versatility and multifunctionality creates attention in the research field related to its applications. A wide number of synthesis techniques also been developed by which ZnO can be grown in different nanoscale forms and thereby different novel nanostructures can be fabricated with different shapes ranging from nanowires to nanobelts and even nanosprings. Generally, nanobelts of ZnO can be obtained by sublimation of ZnO nanopowder without any catalyst. Each property of ZnO has its own applications. Starting from the wide band gap of ZnO makes it enable to form clusters consisting of ZnO nanocrystals and ZnO nanowires.Also due to the wide band gap, synthesis of P–N homojunctions has been reported in some literatures but clarity on stability and reproducibility has not been established yet.

Many fine optical devices can be fabricated based on the free-exciton binding energy in ZnO that is 60 meV because large exciton binding energy makes ZnO eligible to persist at room temperature and higher too. Since ZnO crystals and thin films exhibit second- and third-order non-linear optical behaviour, it can be used for non-linear optical devices. Third-order non-linear response has recently been observed in ZnOnano -crystalline films which make it suitable for integrated non-linear optical devices.

Generally,the advantage of tuning the physical property of these oxides like zinc oxide becomes the root cause for the synthesis of smart application device. the electrical, optical, magnetic, and chemical properties can be very well tuned by making permutation and combination of the two basic structural characteristics they possess the is cations with mixed valence states, and anions with deficiencies(vacancies). Thus, making them suitable for several application fields such as semiconductor, superconductor, ferroelectrics, and magnetic. DSSCs is an optoelectronics device that converts light to electrical energy via charge separation in sensitizer dyes absorbed on a wide band gap semiconductor, which is different to conventional cells[23]. One important difference between conventional and dry sensitized solar cell is that they are epitomized by silicon p-n junction solar cells. The demand for zinc oxide based dye-sensitized solar cell is due to its low fabrication cost.

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