IJCRT.ORG ISSN : 2320-2882

INTERNATIONAL JOURNAL OF CREATIVE RESEARCH THOUGHTS (IJCRT)

An International Open Access, Peer-reviewed, Refereed Journal

A Broad Review Of Properties Of Cerium Based Rare Earth Metals With Respect To Ab Initio And Density Function Theory

1Monika Nagrani, 2Dharamveer Singh

1Research Scholar, 2Professor

1MONIKA NAGRANI,

2B.R.Ambedkar University

Abstract : Rare earth extraction is difficult part of isolating as they were incorporated with many problems. Most of the Rare earth do not get isolated ,either they crystallise and form compounds at normal temperature or pressure .Out of them, Cerium nitride is one of the most required and essential whose important parameters of different properties gets evaluated as per Ab Initio and Density Function Theory. So ,it would lay down a strong ground for cerium based compounds.

Keywords: Rare earth metals,Ab Initio Theory,Density Function Theory,Cerium Based Compounds.

Author:MONIKA NAGRANI (Research Scholar, Agra college),+919368729115, DR D.V. SINGH(Professor Agra College, Agra college)

Introduction: Metals form an important class of technological materials and have to be imbibed with different electronics, mechanical, thermal and optical properties. They are important because of their interesting, semi conducting properties and various application. In the field of alloys and electronic Crystal Ionicity , cohesive energy, heat of formation, bulk modulus and crystal structure which are important parameter and used to highlight its electronic properties(1).

All the rare earth extraction Chalcogenides and pnictides are difficult to fabricate so frequent so repeated practices were incorporated.

Phillip et al and Van Vachten et.al calculated homopolar and hetropolar energy gaps with reference to seperate energy gap (2,3,4).Levine et.al later elaborated Phillip and other theories of complex structured compounds with respect to the d core electrons(5,6,7).From above theory it was deduced that homopolar energy gap being at the nearest neighbouring distance, denoted by E_h while hetropolar energy gap E_C in terms of interatomic distance uses the power law.Singh et.al moreover elaborated Levine theory(8). further investigations include homopolar energy Ionic gap and the average energy gap along with electron polarizability. By this we can understand different relations of Rare Earth Monopcnitides , more deeply .Plasmon energy of metal changes when undergoes chemical combination and forms a compound with

them(9,10). Plasmon where is a collective excitation of conduction Electron in a metal and depends on the density of the conduction electrons involving density functional theory broadly.

Theory: on account of above theory, contributions are made with heteropolar energy gap and homopolar energy gap along with average energy gap and are calculated (11-13)

$E_g^2=E_h^2+E_c^2$ -------1

Crystal ionicity can be defined by

$F_i=E_c^2/E_g^2$--------2

Covalent part (E_h)of homopolar energy gap depends on nearest neighbour separations d_{AB}

$E_h=Ad_{AB}^{-K_1}$-------3

Where A and K_1 are constants

$A=40.468\ ev(A^o)^{-2.5}$--------4

$K_1=2.5$

$E_c=be^2(Z_A-Z_B)\ e^{(-K_s d_o)}/d_o$--------5

Where Z_A and $Z_B$are valence state of atoms A and B

Where K_s=Thomas Fermi Screening Parameter

$d_o=d/2$;d=neighbouring distance

b= adjustment parameter as per coordination number around the element

$b=0.089N_c^2$--------6

N_c=Average coordination number

b=3.204

Bulk Modulus(B)=$M(\hbar\omega_p)^{2.33}$---------7

Optical Suceptibility(X)=$N(\hbar\omega_p)^{-1.33}$-------8

Where M and N are constants that depend on crystal structures.

($\hbar\omega_p$)=Plasmon Energy in eV so we can calculate above parameters with respect to Plasmon Energy

$E_h=D(\hbar\omega_p)^{1.667}$------9

$Ec=S(\hbar\omega p)1.333$----------10

$E_g=Y(\hbar\omega_p)^{1.413}$--------11

$F_i=D^x(\hbar\omega_p)^{-0.16}$-------12

$X_e=S^x(\hbar\omega_p)^{-2.826}$--------13

Where D=0.308,S=0.089,Y=0.094,D^x=0.894,S^x=19934.75

According to electron model

$E_p=\hbar\sqrt{ne2/meo}=\hbar\omega_p$-------14

n=conduction electron density

e=electronic charge

m=electronic mass

$€_o$=Permittivity of free space

ħ=reduced plank constant=$1.0543*10^{-34}$jsec

$ω_p$=Plasmon frequency

Among rare earth compounds nitrides of rare earth are an interesting group of material for theoretical and deductive challenges .These materials brings relation between magnetic and electronic properties . The rare earth nitrides lies on boundary between metal and insulators . Most of Rare earth metals do not get isolated as they are found in compounds most often . Rare earth nitrides crystallise in Rock salt structure at normal temperature (17,18)

First and foremost is cerium nitride and as per reported theoretical calculations were primarily based on ab initio calculations , which has been proposed with the treatment of 4f states for the metal .The lattice constant and bulk modulus of rare earth nitrides have also been reported . Cerium nitride has some unusual properties compared with other rare earth nitrides .The pressure induced structural phase transition of cerium nitride thus is an interesting topic of research and evaluation of First principle calculations of various properties of rare earth nitrides is required.

Foremost compound of this series is cerium. The chemistry of Rare earth elements is largely determined by ionic radius which decreases steadily, corresponding with filling of 4f orbitals . The pressure induced structural phase transition of CeN is an interesting topic of research .Very little theoretical and experimental work has been reported on its structural , magnetic , electrical and optical properties till now .

Danan et Al (19) studied temperature dependence of lattice constant and magnetic susceptibility of cerium nitride compounds . Suane et Al (20) conducted bulk modulus calculations of cerium nitride .Rukmangal et .al(21) proposed structural and elastic properties under high pressure of cerium nitride and have been investigated using two body potential theory with ionic modified charge . Lee et Al investigated epitaxial layer of cerium nitride on magnesium(001) in detail.kanchan et.al(22) investigated and proposed Lattice dynamics and elastic properties of CeN using ab initio density function methods.As per data CeN has not much been the area of research so, all above calculations were based on ab initio theory.But on the basis of DST theory few more calculations have been made with generalised gradient approximation within treatment of 4f states.

DST and Ground state properties:

After obtaining equilibrium lattice constant(a),Bulk modulus(B) and pressure derivative (B_1) and minimum equilibrium volume (V_o)

$P(V)=B/B'[(V_o/V)^{B'}-1]$.....(15)

$B=-V\frac{\partial P}{\partial V} = V\partial^2 E/\partial V^2$.....(16)

$B'=\frac{\partial P}{\partial V}$ ... ... (17)

Many Structural properties like enthalpy etc have been found by performing calculations on electronic band structures so that total energy of cerium nitride can be calculated.while elastic properties of elastic materials are closely related to specific heat thermal expansion,Deby temperature.A material said to be of anisotropic value of a measurement as varies with direction.

$G_V=(2C+3C_{44})/5$……(18)

$G_{R=}15(16/C+9/C_{44})^{-1}$…..(19)

$C=(C_{11}-C_{12})/2$…..(20)

G_V=Voigst Shear Modulus

G_R=Reverse Shear Modulus

Y=9BG/(3B+G)-------(21)

A=Elastic Anisotropic parameter

$A=2C_{44}/C_{11}-C_{12}$…..(22)

$\sigma = (3B - 2G)/(6B+2G)$…..(23)

The brittle/ductile nature of CeN can be determined by ratio(B/G).if (B/G) >1.75 it is more of ductile nature

Table: cerium nitride values(approx)

Approx.	C_{11}	C_{12}	C_{14}	C_{12-44}	G	Y	A	σ	B/G
2.99	315.0	73.3	772	-3.7	92.41	231.42	0.633	0.249	1.666

Conclusion: Thus cerium based compounds has been one of the most important material to be investigated.More properties and usage if investigated can be helpful and beneficial in times to come.Out of all other rare earth compounds cerium based compounds as per there usage in wide applications can be highly beneficial and uphold top position among other rare earth compounds.So research could be profoundly alleviated if focussed on cerium and cerium based compounds.

REFERENCES:

(1)Levine B.F. and Levine B.F.(1973),Phys.Rev B72591,Phys.Rev B72600.

(2)Phillips J.C.,(1968).Phys Rev Lett,20:550.

(3)Phillips J.C.,(1970),Rev.Mod.Phys,42:317

(4)Phillips J.C. and Van Vanchten J.A.(1969),Phys.Rev.183709.

(5)Levine B.F. and Levine B.F.,(1973),Phys Rev B72591 and Phys Rev B72600,193

(6)Levine B.F., J.Phys .Chem 59:463 .

(7) Levine B.F.,(1970), Phys.Rev.Lett 2544.

(8)Singh B.P.,Ojha A.C. and Tripti S.,(2004),Physica B.,350-338.

(9)Shrivastav K.S.,Srivastav R.L. and Harsh Okand kumar V.,(1974),Phys.Rev.B194336.

(10)Srivastav K.S.,Srivastv R.L.,Harsh O.K. and Kumar V.J.,(1979),Phys.Chem,Solids40489.

(11)Singh O.P.,Gupta V.P.,(1985),Phys Stat Sol(b),29:153.

(12)Singh D.V. and Gupta V.P.,Phys.Stat.Sol(b),171.

(13)Singh O.P and Gupta V.P.,(1986),Phys.Stat.Sol(b),137:97.

(14)Yadav D.S. and Singh D.V.,(2012),Phys.Scr.85015701.

(15)Yadav D.S. and Kumar J.,(2012),Computer Innovation,3(2):26.

(16)Chemla D.S.,(1971),Phys. Rev.Lett.26:441.

(17)Larson P,Laubrecht W.R.L.,Chantis A., and Schiff Gaarde Van M.,(2007),Phys.Rev.B,75045114.

(18)Preston A.R.H,Granvile S.,Housden D.H.,Lubrook B,Ruck B.J. and Trodahl H.J.,(2007),Phys.Rev.B.,76,245:120

(19)Danan J.,Novion D.E.C. and Lallemen R.,(1969),Solid State Commun,7:1103.

(20)Svane A.,Szotek Z.,Temmermen W.M.,Laqsquacerd J., and Winter H.J.,(1998),Phys.condens.Mat,10:5309

(21)Ruckmangad A.,Anayes M.,and Sansya L.S.P.,(2009),Indian J.Pure.Ap Phys,47:114.

(22)Kanchana V.,Vatheswarna G.,Zhang X.,Ma Y.,Svane A.,and Eriksson O.,(2011),Phys Rev B,841:205135