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SOME THEORETICAL ANALOGIES IN THE DESCRIPTION OF STRUCTURAL AND MECHANICAL PROPERTIES OF ABO3 TYPE PEROVSKITE MATERIAL

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ABSTRACT

The result obtained using Experimental approaches, Computer based Approaches, Physical Method approaches, Statistical Method approaches to investigate structural properties of ABO3 type perovskite oxides are widely used in last two decades and results so found vary from one approach to another approach. Therefore it is felt that a theoretical unified approach may resolve the variation in the results obtained by different approaches and can predict the actual existing values of structural properties of the materials under investigation. Therefore we have employed a theoretical approach to understand the trends and values regarding structural properties of the above said compounds.

KEYWORDS: Elastic constant, Crystallographic Ratio. Refractive Index, Specific Heat, Conductivity, Polarizability. Electronegativity.

INTRODUCTION

Perovskite is one of the most frequently encountered structures in solid-state physics, for last few years and it accommodates most of the metallic ions in the periodic table with a significant number of different anions. The lattice distortions give rise to many changes of the microscopic and the macroscopic properties, such as bonding mechanism, charge distribution, electronic structure and spontaneous polarization, etc. Therefore, a large number of theoretical and experimental researches have focused on the effects of lattice strain and ion displacements in the ferroelectric perovskite materials [1-4]. Those studies have demonstrated successfully the changes of the properties of perovskite, such as dielectric permittivity, piezoelectricity, pyroelectricity and spontaneous electrical polarization, according to the lattice strain and the ion displacements [5-6].

In modern high-speed computer techniques, they allow researchers to investigate many structural and physical properties of materials only by computation or simulation instead of by traditional experiments. In the theoretical approach, the empirical method is basically used to predict the structural parameters of solids. Empirical relations have become widely recognized as the method of choice for computational solid-state studies. In many cases empirical relations do not give highly accurate results for each specific material, but they still can be very useful. In particular, the simplicity of empirical relations allows a broader class of researchers to calculate useful properties, and often trends become more evident. Empirical concepts such as valence, empirical radii, electronegativity, ionicity and Plasmon energy are very useful. These concepts are directly associated with the character of the chemical bond and thus provide means for explaining and classifying many basic properties of molecules and solids.

With the help of data bases of known structures or models which have physical meaning, certain regularities, such as laws, rules, principles, factors, tendencies or patterns, might be found to help predict unknown structures. The prediction based on correlations is a powerful tool for measuring the association between two variables and for expressing the dependence of one variable on the other, it measures only linear association. Some correlations have a simple theoretical basis while others can be found by empirical methods by an appropriate search routine. These correlations can be classified as three different types: purely empirical, partly empirical but based on some theoretical concept, and purely theoretical. Within these, the first is often unreliable and may not be worthy; the third is seldom adequately developed. The most widely used correlations are of a form suggested in part by theory,

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with empirical constants based on experimental data. Both of above two examples belong to the second kind of correlations.

Thermal expansion coefficients of materials with comparable atomic packing vary inversely with their melting temperatures. This indirect relationship exists because the higher-melting-point materials have deeper and therefore more symmetrical energy wells. Thus, the mean interatomic distances of more strongly bonded materials increase less with a given change in thermal energy. The melting point and bulk modulus are related since both relate to the bonding energy. Hardness and melting point are related because hardness is related to the stress required to separate atoms during dislocation motion. Since larger interatomic forces of attraction imply deeper energy wells, materials with high melting points are the harder materials, such as diamond, Al_2O_3 and TiC. The correlation holds for materials with weaker bonds. However, there are exceptions to these generalizations when more than one type of bond is present, such as graphite and polyethylene. The relationship between permittivity and refractive index at the level of electronic polarization is another good example.

RESEARCH METHODOLOGY

Statistical tools

The lattice constant values for perovskitc materials is of great importance, owing to the development of new materials designed for different applications, such as ferroelectric thin films, microwave and semiconductor technologies etc. [7, 8]. In general, lattice constant can be measured using X--ray, electron or neutron diffraction techniques; however, it is usually a complicated, difficult and time-consuming process. Advances in high performance computing techniques allow materials to calculates lattice constant based on first-principles quantum mechanism [50]. However, it is still a computing intensive job which may not be within the reach of the majorities due to either a lack of computing resource or computational skills.

Recently, various models have been established that can predict lattice constant of perovskites from selected atomic properties of their structural parameters as follows:-

1) On the basis of a bond-valence method, Lufaso and Woodward [9].
2) The methodology developed by Jiang et. al. [10] which allows one to predict the lattice constants of cubic perovskites by using the known ionic radii of the cations and anion appears to be very useful and should likely become a key reference for materials scientist and engineers working in the field [11, 12].
3) Chen and his collegues [13] used a pattern recognition/ atomic parameter method to find the regularities of the formation and the lattice distortion of perovskites. Their results showed that the lattice constant of cubic perovskite oxides it linearly correlated to the ionic radius, valence electrons and electronegativities of constituent elements.

Data sources-scope and coverage:

It would be of interest to give an alternative explanation for bulk modulus of $MgSi0_3$ perovskite solids at different pressure and volume at various constant temperatures.

The electronic and optical properties of $BaTiO_3$ and $SrTi0_3$ have been measured extensively and accurately [14, 15, 16]. However theoretical treatment of the above properties is lagging behind the measurements. There are several first principles methods available for the calculation of band structures and optical constants of $BaTi0_3$ and $SrTi0_3$. As far as the previous studies of the electronic structure of the present materials are concerned, Mattheiss el. al. [17] performed non self onsistent linear combination of atomic orbitals calculations, and Pertosaet. al. [18] modified the LCAO method density of states (DOS) with experiment. Perkins et. a1. [19] have also calculated the DOS and dielectric function assuming a constant matrix element using the LCAO method.

Oxide perovskites are popular in major industrial applications due to diverse physical properties [20]. Within this family of materials, most of them have the chemical formula ABO_3 when A is a relatively large cation with different valence siting at the corners of the unit cell, B is relatively small cation sitting at the center of the unit cell and O is the anion sitting at face centered position. This class of materials has great potential for a variety of device applications due to their simple crystal structures and unique ferroelectric and dielectric properties. Ferroelectric perovskite materials have been drawing wide spread attention in recent years for their potential applications in the domain of microelectronics and the photo-electron industry.

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RESULTS AND CONCLUSION

With the help of data bases of known structures or models which have physical meaning, certain regularities, such as laws, rules, principles, factors, tendencies or patterns, might be found to help predict unknown structures. The prediction based on correlations is a powerful tool for measuring the association between two variables and for expressing the dependence of one variable on the other, it measures only linear association. Some correlations have a simple theoretical basis while others can be found by empirical methods by an appropriate search routine. These correlations can be classified as three different types: purely empirical, partly empirical but based on some theoretical concept, and purely theoretical. Within these, the first is often unreliable and may not be worthy; the third is seldom adequately developed. The most widely used correlations are of a form suggested in part by theory, with empirical constants based on experimental data. Both of above two examples belong to the second kind of correlations.

Thermal expansion coefficients of materials with comparable atomic packing vary inversely with their melting temperatures. This indirect relationship exists because the higher-melting-point materials have deeper and therefore more symmetrical energy wells. Thus, the mean interatomic distances of more strongly bonded materials increase less with a given change in thermal energy. The melting point and bulk modulus are related since both relate to the bonding energy. Hardness and melting point are related because hardness is related to the stress required to separate atoms during dislocation motion.

Since larger interatomic forces of attraction imply deeper energy wells materials with high melting points are the harder materials, such as diamond, Al_2O_3 and TiC. The correlation holds for materials with weaker bonds. However, there are exceptions to these generalizations when more than one type of bond is present such as graphite and polyethylene. The relationship between permittivity and refractive index at the level of electronic polarization is a other good example. Some conclusion of binary correlations among materials properties are

1. Koh and Kumar et al. have attempted to correlate different physical parameters of compound semiconductors and alkali halides using linear relationships. Koh and Nag have been demonstrated a linear relationship between second order elastic constant and crystallographic ratio for alkali halides.
2. Neumann has proposed the expression for average thermal expansion coefficient for binary tetrahedral semiconductors.
3. Lorentz–Lorenz in 1880 describe dielectric constant 'ε' and refractive index '*n*' at optical frequency with the following relation
   $\sqrt{\varepsilon} = n$

Moss in 1950 made a proposal on the very general ground that all energy levels in a solid are scaled by a factor, $1/\varepsilon_{opt}^2$. Where $\varepsilon_{opt} = n^2$ is the optical dielectric constant. Moss succeeded in systematizing the extensive experimental data on the well-known materials and proposed a relation between the high frequency refractive index and the wavelength the materials.

For a class of semiconductor and others, Moss has proposed a relation, which reads as follows:

$n^4 Eg = 173$ eV

where 'n' is the high frequency refractive index (Eg) is energy gap.

(4) Duffy has introduced the concept of optical electronegativity and its uses in estimating many physico-chemical parameters of materials. The correlation between energy gap and optical electronegativity has been evaluated by Duffy in various binary systems.

(5) The specific heat and atomic/molecular mass: specific heat is a measure of the heat energy required to increase the temperature of a unit mass of a substance by a unit temperature. The heat energy arises, partly due to the number of atoms or molecules that are vibrating and if a substance has a lower molar mass, then each unit mass has more atoms or molecules available to store heat energy.

(6) Specific heat and density in solids: they are related because atoms differ greatly in mass but little in size, and so the density of a solid is mainly determined by its atomic weight and to a lesser degree by atom size and the way in which they are packed. Because of this correlation between density and atomic weight and the correlation between atomic weight and specific heat capacity, there is a strong, inverse correlation between density and specific heat.

(7) Electrical and thermal conductivity in metals: The electronic theory of Drude explained Lorenz's relation on the assumption that both heat and electric currents in matter results from the motion of its electrons. According to Drude's theory, the value of the temperature-dependent Wiedemann-Franz constant (i.e. the Lorenz number) is

$$L = \frac{\kappa}{\sigma T} = \frac{\pi^2}{3}\left(\frac{\kappa^2}{\varepsilon}\right)$$

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where L is Lorenz number, κ is thermal conductivity, σ is electrical conductivity, T is temperature; k is Boltzmann's constant, and ε is the charge of an electron. In general, the Lorenz number L, while roughly constant, is not exactly the same for all materials; Kittel gives some values of L ranging from $L = 2.23 \times 10^{-8}$ W Ω K^{-2} for Cu at 0 ºC to $L = 3.2 \times 10^{-8}$ W Ω K^{-2} for W at 100 ºC.

(8) Guo et al. have identified the relation between the ionicity of binary oxides and the cation radius and extended that to estimate the ionicity and molar refraction for a wide range ofoxides and silicates.

(9) Electronic polarizability of different crystals has been calculated by several authors using the dielectric theory of Phillips and Van Vechten and the bond charge model of Levine.

Other several binary correlations are proposed between bulk modulus, microhardness, ionicity, surface energy, melting point, Debye temperature, bond length, Plasmon energy, nuclear effective charge, refractive index and energy gap for variety of materials. Significant theoretical work has been done in this direction for various materials.

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