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STUDY ELECTRONIC PROPERTIES OF THE IDEAL PEROVSKITE STRUCTURE

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ABSTRACT

The ideal ABO_3 *perovskite structure is cubic (space group Pm_33m) and is composed of a three-dimensional network of vertex-sharing* BX_6 *octahedra. The A-site cation fills the 12- coordinated cavities (cuboctahedra) of the three-dimensional network. This structure is very flexible and it can accommodate most of the metallic elements of the periodic table. Depending on the ionic radii of A and B, octahedral are tilted, thus reducing the volume of the cub octahedron until it fits the size of the A cation. The highly versatile* ABX_3 *perovskite crystal structure is formed by the B cations filling 25% of the octahedral holes in the cubic close-packed* AX_3 *array. In the ideal cubic structure, each A cation is coordinated to twelve X anions and each B cation is coordinated to six X anions. An example of the ideal cubic structure is* $SrTiO_3$*.*

Keywords: Electrical Resistance, Low Temperatures, Strong Magnetic Field.

I. INTRODUCTION

The perovskite structure class is one of the most commonly occurring and important in all of materials science. Perovskites are ceramics (or rather, electro-ceramics), which constitute the Earth's most abundant mineral group and hold clues to the planet's history. A number of synthetic perovskites are of major technological importance. Barium titanate ($BaTiO_3$) and lead zirconate-titanate (PZT) ceramics form the basis of a sizable industry in ferroelectric and piezoelectric materials crucial to transducers, capacitors, and electronics. The perovskite structure occupies a prominent place under all the known ternary systems of composition ABX_3. This is due not only to its wide occurrence, but also to a series of interesting and useful properties associated with this structural type.

The ideal ABO_3 perovskite structure is cubic (space group Pm_33m) and is composed of a three-dimensional network of vertex-sharing BX_6 octahedra. The A-site cation fills the 12- coordinated cavities (cuboctahedra) of the three-dimensional network. This structure is very flexible and it can accommodate most of the metallic elements of the periodic table. Depending on the ionic radii of A and B, octahedral are tilted, thus reducing the volume of the cub octahedron until it fits the size of the A cation. Tilting of octahedra reduces the symmetry of structure. Analysis of perovskite-related structures has shown that in many cases the BX_6 octahedra are distorted, which may be a cause for the reduction of symmetry by itself. There are many ways in which the octahedra can tilt and distort, each leading to a different symmetry .The highly versatile ABX_3 perovskite crystal structure is formed by the B cations filling 25% of the octahedral holes in the cubic close-packed AX_3 array. In the ideal cubic structure, each A cation is coordinated to twelve X anions and each B cation is coordinated to six

X anions. An example of the ideal cubic structure is shown in Figure 1. The substitution of different atoms into the A and B positions is possible if they are of similar size to A and B respectively, and total equivalent oxidation state.

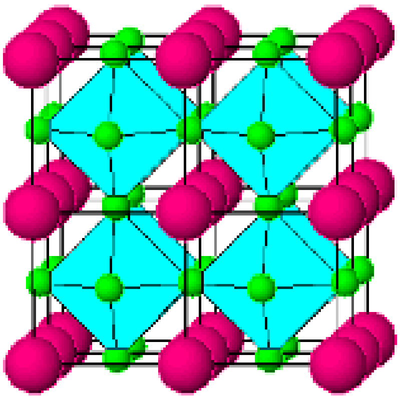

Figure 1: An ideal cubic perovskite $SrTiO_3$ with Pm-3m symmetry

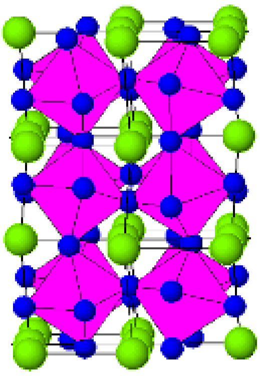

Figure 2: A distorted perovskite $SmNiO_3$ with orthorhombic symmetry.

Most perovskite structures are distorted and do not have cubic symmetry. Common distortions such as cation displacements within the octahedra and tilting of the octahedra are related to the properties of the A and B substituted atoms. Factors that contribute to distortion in the structure include radius size effects and the Jahn-teller effect. The $SmNiO_3$ structure shown in Figure 2 is a distorted perovskite with orthorhombic symmetry. The distortions exhibited by perovskites as a consequence of cation substitution can be used to fine tune and adjust properties of interest. A few of the physical properties of interest in various perovskite systems include conductivity, dielectrics, and colossal magnetoresistance. The following subsections contain examples of perovskite type structures and explanations of their properties and relations to the ideal perovskite structure.

II. REVIEW OF LITERATURE

Due to the increasing technical importance of several perovskite-type materials, a number of books, monographs and review articles on different aspects of their structural characteristics and properties have been published in recent years and the pertinent sections. So it becomes very difficult to summarize the available information in a reduced space such as that available here. At present, environment-friendly and efficient technologies are doing put into practice at an ever increasing rate and for their adequate implementation;

III. MATERIAL AND METHOD

CRYSTAL CHEMISTRY OF THE PEROVSKITE STRUCTURE

3.1 The ideal perovskite structure

The structure of an ideal cubic ABX_3-perovskite is usually depicted schematically. A being the larger cation, B the smaller one and X the anion. This anion may be oxide, fluoride and, in a few cases, chloride, bromide, iodide, sulphide or hydride. In this article we will concentrate mainly on oxide systems. The structure can be related also, in a direct way, to that of $Re0_3$. For an ideal perovskite, t is unity; however, the perovskite structure is also found for lower t-values (0.75 < t S 1). In such cases, the structure distorts to tetragonal, rhombohedral or other lower symmetries. Indeed, many perovskitic oxides are polymorphs. Moreover, the above given geometric relations are not a sufficient condition for the stabilization of the perovskite lattice, since the A and B cations must, in themselves, be stable in twelvefold (12 or (8+4) or (6+6)) and sixfold coordination respectively. This latter condition sets lower limits for the cationic radii. In oxide systems these limits are rA > 0.90 i and rB > 0.51 I . A typical and well known example of the ideal cubic structure at room temperature is $SrTi0_3$ with a = 3.905 i and space group Pm3m (ref.7), in which the Ti06- octahedra are undistorted with 90" angles and six equal Ti-0 bonds at 1.952 i. Each strontium ion is surrounded by twelve equidistant oxygen atoms at 2.761 i. Some other materials that adopt this ideal structure are $KU0_3$, $KMgF_3$, $SrLiH_3$, $CaI0_3$, $SrZr0_3$, $SrHf0_3$, $BaSn0_3$, $TlMn0_3$, $NH4CoF_3$, $BaCe0_3$, $ZnNiF_3$, $LaMn0_3$, etc**.** . It is interesting to remark that many compounds present the ideal cubic structure only at high temperatures, and generally this high-temperature form cannot be quenched

3.2 Tetragonal Perovskites

The best known example of a tetragonal perovskite is probably the room temperature form of the ferroelectric $BaTi0_3$, with a = 3.994 A°, c = 4.038 A°; and Z = 1. In this case the TiO_6-octahedra are somewhat distorted (one Ti-0 bond at 1.86 i, four at 2.00 I and one longer at 2.17 i). Barium is coordinated by four oxygens at 2.80 A°, four at 2.83 A° and four more at 2.88 A°. In the isotypic $PbTi0_3$, the TiO_6-polyhedra are more distorted than in $BaTi0_3$, a fact which can surely be related to the greater polarizino power of Pb(II), which has often been discussed in relation to other structural and bonding problems in systems containing this cation .A number of other tetragonal perovskites ($PbHf0_3$, $SrPb0_3$, $SrZr0_3$, $AgTa0_3$, $KCoF_3$, $CsPbC1_3$, $CsPbBr_3$,etc.) are isotypic with $BaTi0_3$ and possess unimolecular cells. The fact that most of them are tetragonal only at high temperatures makes accurate crystallographic studies very difficult. In some cases, more complex tetragonal unit cells have been found; also superstructure reflections can be observed in some tetragonal perovskites, pointing to multiple cells or to cells of lower symmetries . $KCuF_3$ has a tetragonal superstructure due to a shift of thefluoride ions, caused by the Jahn-Teller effect. As expected, the CuF_6-octahedra are elongated, with two significantly longer Cu-F distances   **.**

3.3 Rhombohedral Perovskites

In several materials the cubic cell may have a small deformation to rhombohedral symmetry. If this deformation does not enlarge the unit cell, it is possible to index it on a unit cell containing either one or two formula units with rhombohedral angles cr~90° or ad60 respectively. However, the anions are generally displaced as requires the larger unit cell with aa60'. Examples of rhombohedral perovskites are $LaA10_3$, $PrA10_3$, $LaNi0_3$ and $LaCoO_3$. $LaCoO_3$ has this rhombohedral structure at room temperature, but at higher temperatures it undergoes two interesting phase transitions transforming to another rhombohedra phase (Rgc to R_3), in which trivalent cobalt is ordered in such a way that there are alternating (111) planes with high-spin and low-spin Co(II1) ions. Above 937°C a second transition occurs, in which the space group R3 is retained but the o-angle drops abruptly from 60.4 to 60^0.

3.4 Orthorhombic Perovskites

The $GdFe0_3$ structure is probably the most common of all the orthorhombically distorted perovskites. Its space group is Pbnm and the cell constants are: a = 5.346 A° i, b = 5.616 A° and c = 7.666 A° with Z = 4. In this structure the $Fe0_6$- octahedra are distorted and tilted. Also the GdO12 - polyhedron is severely distorted, showing an (8+4) coordination. Other materials adopting this orthorhombic-distorted structure are $NaU0_3$, $NaMgF_3$, $LaYb0_3$ and a great number of lanthanide compounds of the type $LnCr0_3$, $Ln3a0_3$, $Ln'Fe0_3$, $Lnqn0_3$, $LnRh0_3$, etc **.**

3.5 Monoclinic and Triclinic Perovskites

Monoclinic ($AgCuF_3$, $CsPb1_3$, $PbSn0_3$, $BiCr0_3$, etc.) or triclinic (BiMn03, $BiScO_3$) unit cells have been reported in several cases. However, in many cases these cells have proved to be pseudo cells of a real multiple cell. For example, ; $dFe0_3$-type phases have been frequently indexed on the bases of a monoclinic DSeUdOCell with a%bscQa' and Bs90.

IV. RESULT AND CONCLUSIONS

4.1 Accordingly, the main objectives of our research paper are

A. To collect a set of new experimental data on various electronic properties such as transducers, capacitors, ionic radii, Cyrstal structure for the perovskite structure.
B. To evaluate various excess electronic functions for the individual properties from the measured data on.
C. To understand the recent various existing theories of perovskite structure based on statistical with the experimentally derived properties to the perovskite structure.
D. To understand the complex molecular interactions in the perovskite structure from the knowledge of corresponding experimental data.
E. To develop models with for prediction of electronic properties of such perovskite structure.

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