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STUDY OF FORMABILITY IN CUBIC PEROVSKITES OXIDES

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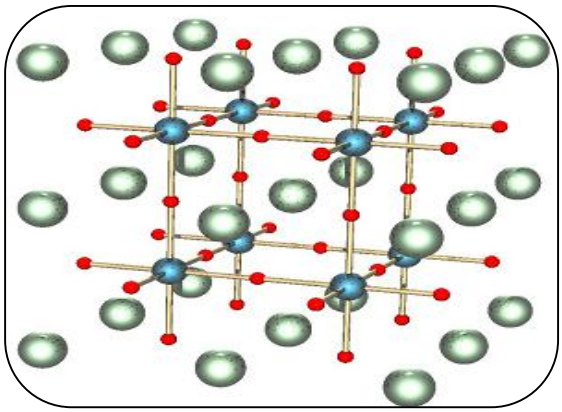

ABSTRACT

Perovskite is one of the most frequently encountered structures in solid-state physics, and it accommodates most of the metallic ions in the periodic table with a significant number of different anions. In this Paper we have studied some structural properties such as lattice constants, formability of a large no of ABO_3-type Perovskites solids. Megaw determined the structure perovskite by examining high angle lines on X-ray powder photographs. Salinas-Sanchez introduced a parameter called the global instability index (GII), which can be used to determine the overall structural stability of perovskite. Giaquinta and Loye predicted the perovskite structure based on the combination of ionic radii.

KEY WORDS - *X-ray powder photograph, periodic table, significant number, global instability index (GII), etc.*

INTRODUCTION-

The study of ABO_3 compounds has a long history. Megaw accurately determined the structure of a number of doubled perovskite by examining high angle lines on X-ray powder photographs. Salinas-Sanchez introduced a parameter called the global instability index (GII), which can be used to determine the overall structural stability of perovskite. Giaquinta and Loye later predicted the perovskite structure for a number of compounds based on the combination of ionic radii and bond ionicities, predicting the structure of ABO_3 (A = In, B = Mn, Fe) with this method. Lufaso and Woodward used a bond-valence model to tolerance factor (t_{BV}) which they proposed as a new criterion of the structural stability of ABO_3-type perovskite compounds. Ye *et al.* Applied a pattern recognition method and found some regularity in the formation and the lattice distortion of perovskites. Li *et al.* used $r_A - r_B$ structure maps to study the perovskite formability of 197 ABO_3 compounds by octahedral factor (r_B/r_O) and tolerance factor (t).

REVIEW OF LITERATURE=

During the last few years, many experimental and theoretical investigations were devoted to the study of perovskite solids. Many researchers try to design and synthesize new cubic perovskite used as substrate materials. Obviously, if new cubic perovskite compounds and their lattice constants can be predicted, it will be helpful to design new substrate or buffer materials with cubic perovskite structure. The physical and chemical properties of perovskite and perovskite-related materials are diverse and can be applied in a variety of fields, so it is useful to discover the regularities that govern the formation of perovskite-type compounds in order to guide the exploration of new materials in the huge compositional spaces available. In this Paper we have studied some structural properties such as lattice constants, formability of a large no of ABO_3-type perovskite solids.

MATERIAL AND METHOD=

STRUCTURAL MAP METHOD:

In this paper, we have produced a new modified structure map method for determinations the formability of ABO_3-type perovskite compounds. In these maps the perovskite formation regions are shown clearly, which may help us design novel materials with a perovskite or perovskite-related structure. In 1926, Goldschmidt had used ''tolerance factor'' to study the stability of perovskites. Goldschmidt found that, t values of cubic perovskites are in the range of 0.8–0.9. Goldschmidt's tolerance factor t has been widely accepted as a criterion for the formation of the perovskite structure, and therefore, it is an important factor for the stability of cubic perovskites, so tolerance factor t constructs one axe of the structure map . However, up to now, it seems that t is not a sufficient condition for the formation of the cubic perovskite structure, for example, in many systems whose t are even within the range (0.8–0.9), no cubic perovskite structure is stable, such as, $LaVO_3$, $DyMnO_3$, and $CaMoO_3$. So, another important factor governing formability of cubic perovskite should be introduced. Prediction criterions for the formabilitie of perovskite-type oxides are obtained by using the empirical structure map methods constructed by two parameters octahedral factor (r_B/r_O) and tolerance factor, on this structure map, simple point representing systems of forming and non forming are distributed in distinctively different regions. In this chapter we found that the octahedral factor (r_B/r_O) is as important as the tolerance factor with regards to the formability of perovskite-type oxides. We have applied the proposed model to 173 ABO_3 perovskite and it can be used to search for new perovskite-type oxides by screening all possible elemental combinations.

RESULT AND DISSCUSION=

Mooser and Perason applied a two-dimension graphic to study the stability of different compounds, the two factors they used were the difference of electro negativity between the cation and the anion and the average principle quantum number. They succeeded to discriminate the crystal structures of AB-type compounds, of AX_2-type halides, and the metallic or non-metallic ternary fluorides ABX. Similar methods were called the structural map technology, and more parameters were used to draw the graphic. Muller and Roy proposed to plot ''structural map'', which took the ionic radius of A and B as coordinates to study the distribution of different structures for many ternary structural families. Furthermore, the schematic distribution map of different crystal structure for $A^{+1}B^{+5}X_3$, $A^{+2}B^{+4}X_3$ and $A^{+3}B^{+3}X_3$ systems separately, were given by the same method . However, the criterion for perovskite formability was not discussed, possibly due to the lack of accurate data of crystal structure of some ABX_3 compounds at that time. The ionic radius is the most important ionic parameter that dominates the crystal structure of ionic compound. In this study, the same method will be used to find the regularities governing cubic perovskites formability.

The much used Goldschmidt's tolerance factor (t) is defined as

$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)} \qquad \text{..... (1)}$$

Where r_A, r_B and r_X are the ionic radii of A, B and X_3 respectively

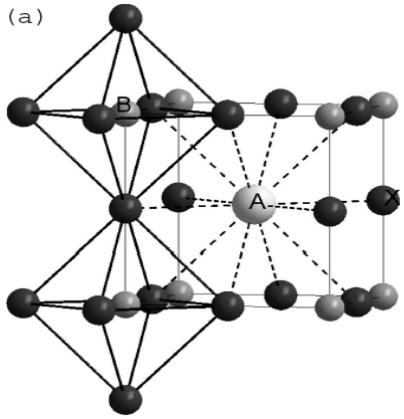

Figure 4.1 (a) Ideal cubic perovskite structure,

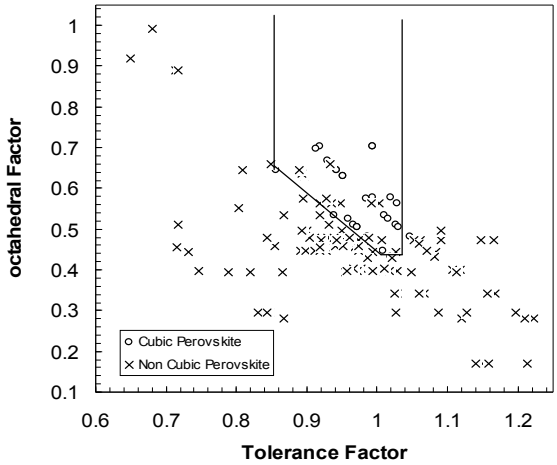

Figure 4.2 Classification of cubic (ABO_3) perovskite oxides

Table 4.1 Values of ionic radius, tolerance factor (t), octahedral factor (r_B/r_X) and formability of 173 perovskite solids.

Solids	r_A(Å) [7,22]	r_B(Å) [7,22]	Tolerance factor (t)	r_B/r_X	Formability*
$CsIO_3$	1.88	0.95	0.993	0.704	F
$CsNbO_3$	1.88	0.64	1.148	0.474	NF
$CsVO_3$	1.88	0.54	1.028	0.341	NF
KUO_3	1.64	0.76	1.002	0.563	F
$KPaO_3$	1.64	0.78	0.993	0.578	F
$KTaO_3$	1.64	0.64	1.062	0.474	F
$KNbO_3$	1.64	0.64	1.062	0.474	NF
$KAsO_3$	1.64	0.46	1.168	0.341	NF
KVO_3	1.64	0.54	1.119	0.400	NF
KPO_3	1.64	0.38	1.222	0.281	NF
$KSbO_3$	1.64	0.60	1.084	0.444	NF
KIO_3	1.64	0.95	0.919	0.704	F
$KBiO_3$	1.64	0.76	1.002	0.563	NF
$NaTaO_3$	1.39	0.64	0.974	0.474	NF
$NaAlO_3$	1.39	0.535	1.028	0.396	NF

CONCLUSION:

Through study of formability in cubic perovskite, the following conclusions are obtained:

1. In the R_A-R_B structural map the systems with perovskite and those non perovskite are distributed in distinctively different regions; there exists a clear boundary between these two kinds of samples.
2. Octahedral factor is as important as the tolerance factor for cubic perovskite formability.
3. Both tolerance factor (t) and octahedral factor (r_B/r_O) are a necessary but not sufficient condition for cubic Perovskites formability. Using these two factors, the cubic Perovskites formability can be reliably predicted.
4. In the structural map that is drawn by the tolerance factor and octahedral factor (r_B/r_O) the points for cubic Perovskites and those for non-cubic Perovskites are located in different zones via clear boundary defined by Eqs. (1). these equations form the criteria for cubic Perovskites formability.

The simple method presented in this work will be helpful to material scientists for finding new substrate or buffer materials in compound semiconductor epitaxy.

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