Phase Diagram Studies on the Mixed Rare Earth Oxide System (DY_2O_3 & ZRO_2)

- Anitha Sagayapushpam* - A. Christy Ferdinand** - D. Manikandan***

Abstract

The ICDD is a non-profit organization established by a number of international scientific organizations. This organization provides the determination of powder patterns. Most of the patterns published in PDF obtained from useful sources of information for crystal structure. The PDF is a collection of single phase x-ray diffraction patterns in the form of tables of inter planar spacing and corresponding relative intensities. A typical data "card" obtained from the computer version of the PDF.

Keywords: Non-Profit Organisation, Patterns, Diffraction Systems, Inter Planar Spacing

Introduction

Materials are used in every activity of life, living things and non-living things are made of materials. Advances in technology depend increasingly on the development of better materials of greater strength, lightness, safety, electrical conductivity, resistance to corrosion and to heat etc, .

Material Science involves investigating the relationships that exist between the structures and properties of materials [1]. Material Science is a field of science that emphasizes studies of relationships between the microstructures, synthesis, processing and the properties of materials . The materials making up the surrounding world consist of discrete particles having sub-microscopic size .Their behaviour is explained by atomic theories .

Powder Diffraction

The ICDD is a non-profit organization established by a number of international scientific organizations .This organization provide the determination of powder patterns. Most of the patterns published in PDF obtained from useful sources of information for crystal structure. The PDF is a collection of single phase x-ray diffraction patterns in the form of tables of inter planar spacing and corresponding relative intensities. A typical data "card" is obtained from the computer version of the PDF.

Generally, materials are broadly classified as

1. Simple materials.
2. Composite materials.

Composites are materials that occur due to combination of materials in definite proportions. Based on these properties a material falls into one of the following categories.

i. Mechanical properties (strength, ductility etc)
ii. Thermal properties (specific heat, melting point etc)
iii. Magnetic properties (permeability, hysteresis etc)
iv. Chemical properties (chemical composition, acidity etc) Optical properties (reflectivity, refractive index etc)
v. Physical properties.

*Department of Physics, St. Joseph's College of Arts & Science, Cuddalore - 607001, Tamilnadu, India.
**Department of Physics, St. Joseph's College of Arts & Science, Cuddalore - 607001, Tamilnadu, India.
***Department of Physics, Arignar Anna Arts College, Cuddalore - 607001, Tamilnadu, India. email: Christy.ferdinand@gamil.com

According to these properties a material is classified as,

A pure metal consist entirely of atoms of only one element. It has its own unique physical properties such as melting point, boiling point, and thermal or heat conductivity. Example: Fork

An alloy is the intimate combination of two or more pure metals that have been dissolved while molten, one into the other. An alloy could be harder, softer, stronger, less easily corroded and so forth, than the individual metals composing it.

They are chemical compounds of the type metals and non-metals. They are generally good thermal and electrical insulators. They are hard and brittle. Example: Scissors, a glass vase, floor tile, a china tea-cup [1].

They are organic compounds, generally in the form of long chain. They have low density. Example: Spoon, fork, knife [1]

They have electrical properties that are intermediate between conductors (eg: metals and alloys) and insulators (Example: Ceramics and polymers). They are composed of more than one type of materials. Most common and familiar composites is fiberglass, in which small glass are embedded within a polymeric material [4].

Powder Data Analysis

Subsequently, the high purity samples like Baf_2, NaCl, LaB_6, URh_3, UGa_3, Dy_2O_3, CsCl and Tm_2O_3, ZrO_2, KCl, KBr and Se theoretical pattern was generated by using the PCW software [5]. Input parameters like the crystal structure, atom positions were taken from Pearson's Intermetallic Database [6-10]. The computed theta values along with respective hkl values and intensities are used to index the experimentally observed Bragg peaks . Care was taken to compare the intensities of every peak and assign the right hkl value. A graph comparing the experimentally observed theta, intensity and theoretical intensity, calculated difference in both values ($2\theta_{EXP}$-$2\theta_{CAL}$) was prepared for this purpose. The indexed experimental data was fed into NBS*AIDS83 SOFTWARE, in order to get the lattice parameter, cell, volume, figure of merit etc [11]. The output giving the lattice parameter found using the least square fitting method (NBS*AIDS83), volume and the figure of merit.

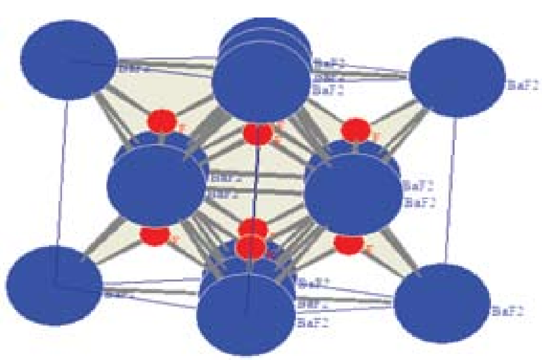


Figure (1) Crystal Structure of BaF_2

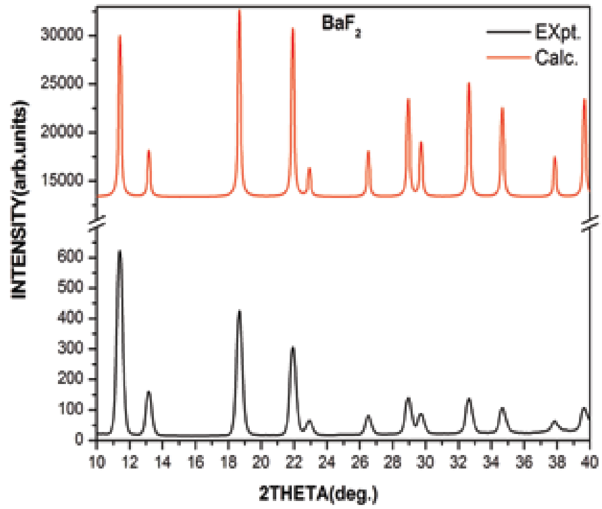


Figure (2) XRD Pattern of BaF_2

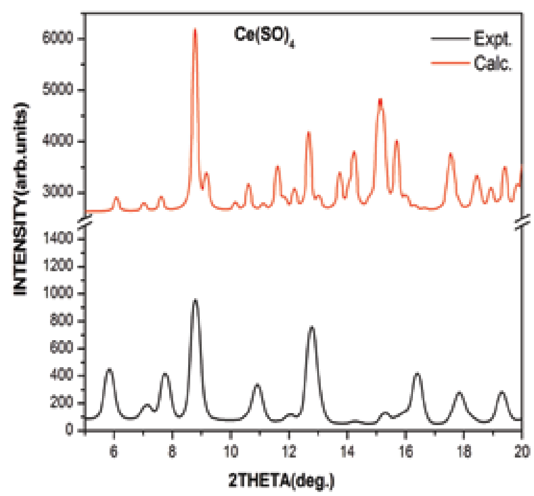


Figure (3.) XRD Pattern Of $Ce(SO)_4$

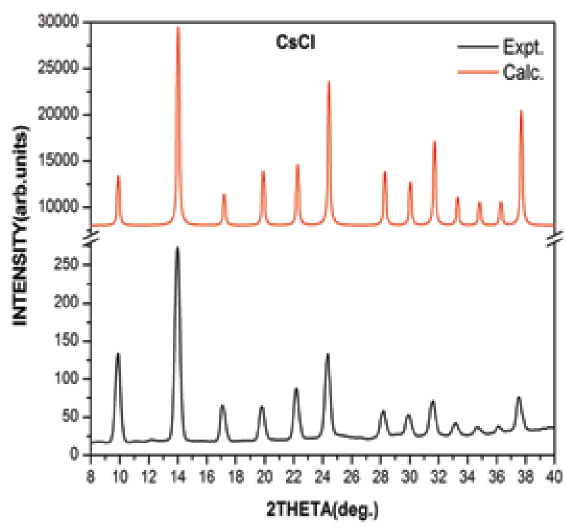


Figure (4) XRD Pattern Of CsCl.

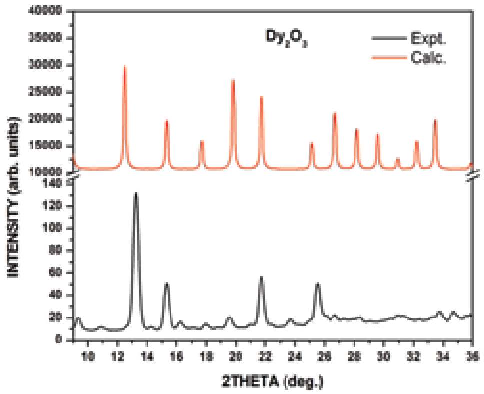
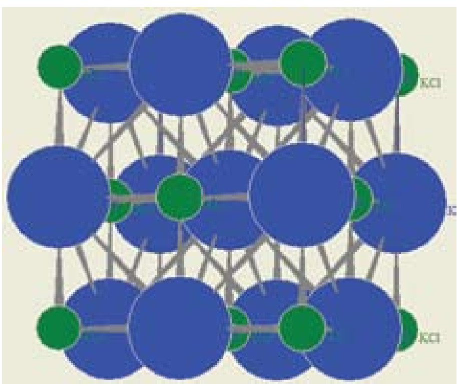


Figure (5) XRD Pattern Of Dy_2O_3



Figure(6) Crystal Structure of KCl

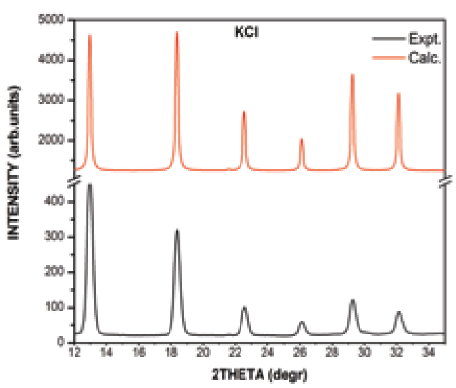


Figure (7) XRD Pattern of KCl

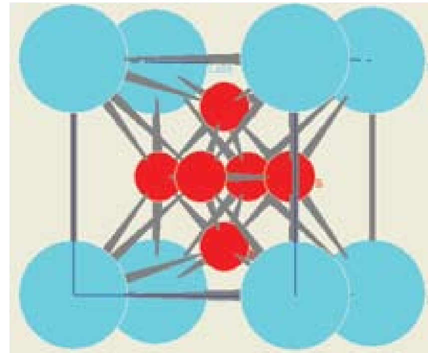


Figure (8) Crystal Sturcture of LaB_6

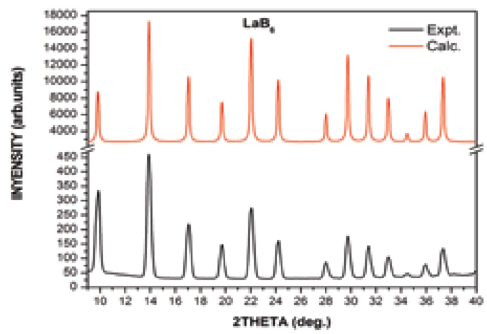


Figure (9) XRD Pattern of LaB_6

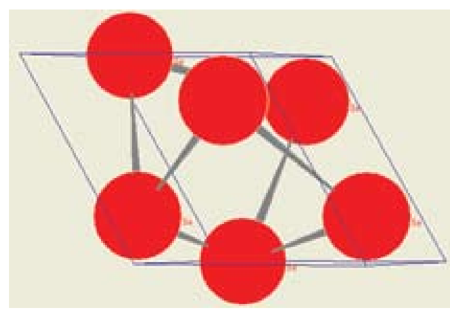


Figure (10) Crystal Sturcture of Se

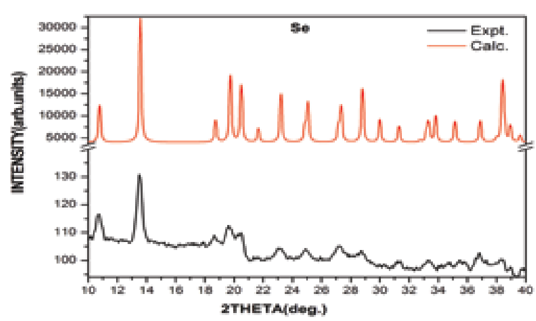


Figure (11) XRD Pattern of Se

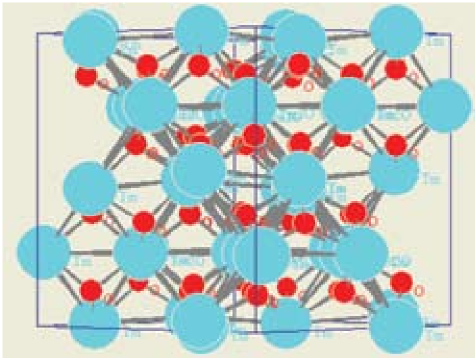


Figure (12) Crystal Sturcture of Tm_2O_3

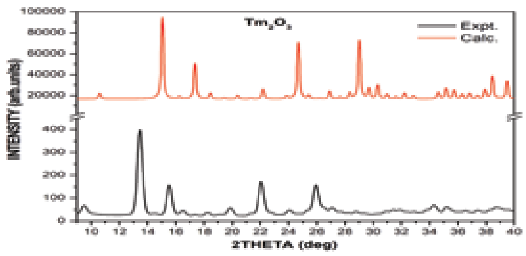


Figure (13) XRD Pattern of Tm_2O_3

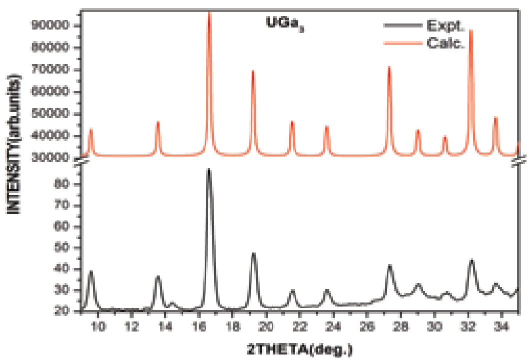


Figure (14) XRD Pattern of UGa_3

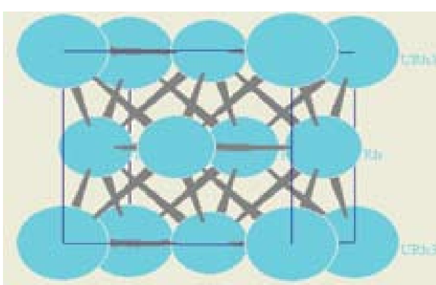


Figure (15) Crystal Structure of URh_3

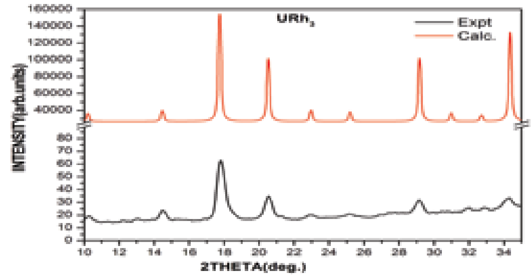


Figure (16) XRD Pattern of URh_3

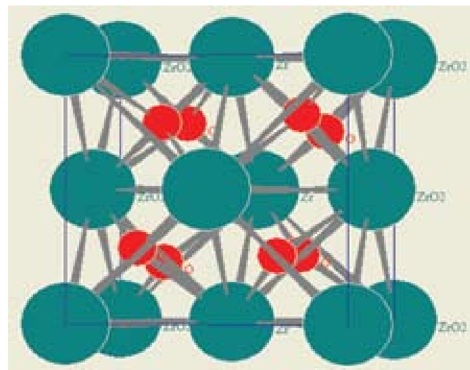


Figure (17) Crystal Structure Of ZrO_2

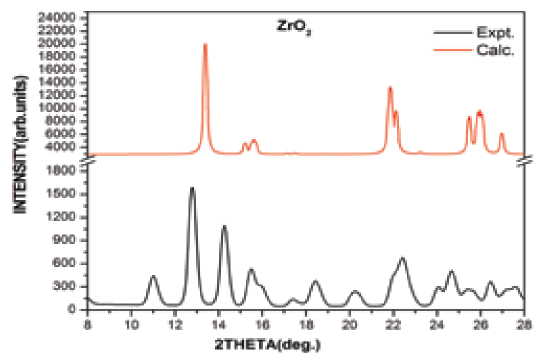


Figure (18) XRD Pattern of ZrO_2

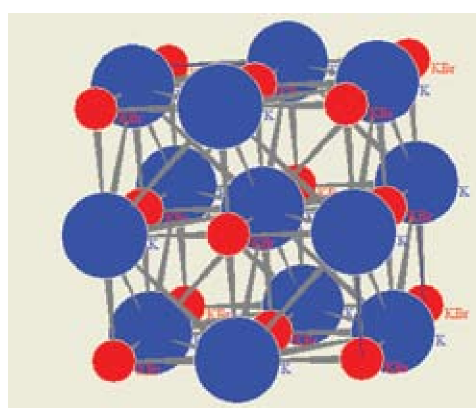


Figure (19) Crystal Structure of KBr

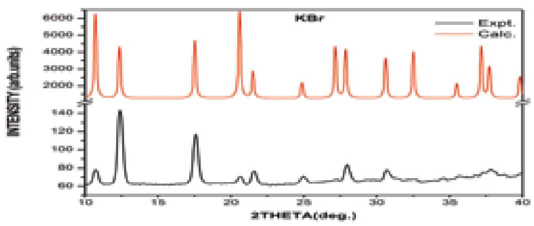


Figure (20) XRD Pattern of KBr

Conclusion

The XRD pattern of mixed oxides ofDy_2O_3 &ZrO_2 were prepared in the pestle and mortar with few drops of hexane. An annealed in the double zone furnace for 12 hours at 1000°C. The compositions vary from 0.9% to 52.9%.From the composition of 0.9%to 10.9% and 42.7% to 50.3% the 100% peak of Dy_2O_3 is visible due to its high intensity. And its peak is very sharp. But from 0.9% to 45.4% the 100% peak of ZrO_2 is not visible, and it is hidden in the shoulder of 100% peak of Dy_2O_3. This is due to low intensity in ZrO_2. In these compositions 21.6%, 32.2% and 52.9%, the 100% peak of ZrO_2 is visible independently due to its high intensity. In these compositions the 100%peak of Dy_2O_3 is not visible, but it is hidden in the shoulder of ZrO_2. This is because of low intensity compared to ZrO_2.

In summary, a high temperature phase diagram studies on the mixed rare earth oxide system (Dy_2O_3 &ZrO_2) was performed. This study reveals their C-type Cubic crystal structure and the B-type Monoclinic at higher temperature. This helps to identify the phase stability. Rare earth oxides Dy_2O_3 &ZrO_2 corrected data were analyzed using NBS*AIDS83, FIT2D&PCW software.

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