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XRD studies of transition metal ions doped in (ZrO2) 0.8 (Y2O3)0.2 ceramic compound

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Summary: ***In this paper, the result of XRD studies in (ZrO2)0.8(Y2O3)0.2 polycrystalline ceramic compound doped with some transition elements are reported in order to investigate their structural and magnetic features. Results will reveal and make us able to discuss in detail that how doped impurities of transition metal ions change the composition of the system along with noticeable.***

Introduction- Stabilized Zirconia has been widely used for many years. The ever increasing applications of oxide in high technology ceramics , particularly in wear parts and as solid electrolytes has attracted a great deal of attention (1). Zirconia ceramics have received considerable attention from the view point of their sintering behaviour and control of the microstructures which develop during sintering process, so that the resulting materials meet the requirements needed for these applications. In order to produce high performance Zirconia ceramics , solid state sintering has traditionally been adopted as the favoured fabrication route. This route has often required the use of high firing temperature for the achievement of high density in Zirconia materials.Several approaches have proved to be effective in reducing these temperatures. Amongst these approaches, the use of reactive powders such as CaO, Y2O3 or rare earths oxides has received particular attention (2). It has been reported that yttria (Y2O3) Stabilized Zirconia compacts sinterd at 12000 C are found to have the highest density (3). Zirconia based coatings are commonly used as thermal barrier coatings (TBCs) are increasingly being employed to provide thermal insulation to critical air - cooled mechanical components of gas turbine engines, thereby improving their efficiency (4). Experimental Study The synthesis of polycrystalline ceramic samples of required stoichiometry in pure as well as doped form has been done using standard high temperature solid state reaction technique. This technique involves grinding of the constituents together followed by pelletization and sintering at high temperature(5).

The transition metal impurities are taken in the form of Cu (NO3) 3H2O, MnCl24H2O and TiO2. A fixed concentration (1wt%) of impurity was added to base ceramic . All the constituents were well mixed together in an agate mortar and pestle then palletised in the form of thin cylindrical pellets under the application of a pressure of 6 ton/cm2. The palletised materials were kept for sintering at temperature of 15500C in a glower furnace for 24 hours. Thus formed materials then characterised through X - ray diffraction (XRD) technique in order to investigate their structural and magnetic properties. The sample code and the composition are given in table-I. The XRD patterns of all the samples were recorded using a Rich Seifert Isodeby flex diffractometer. The recording conditions were scan speed (ss) 30/min, time constant Tc=10 sec., count per minute 5K,and current/ voltage = 20 MA/30KV.

Results and Discussion- fig.(a) shows that the X- ray diffraction (XRD) pattern for sample SZYP. It is evident that the XRD pattern consist of three phases namely , monoclinic, tetragonal and cubic(6). After indexing the observed XRD pattern values are calculated. The observed values of d (dobs), calculated values d (dcal), the millar indices and relative intensities of the peaks are given in table-II. The values of dobs are calculated using Bragg's formula: dobd = Wavelength/2SinA where A is the diffraction angle and dobd is the

interplaner distance.

The values of dcal have been calculated using the following expressions and lattice parameters from literature (7,8) :

For cubic 1/d2cal = (h2+k2+l2)/a2

For tetragonal 1/d2cal = (h2+k2)/a2 + l2/ c2

Fig.(b-d) depict the XRD patterns for samples SZYTi, SZYMn and SZYCu. All samples exhibit essentially the same kind of patterns(9). The percentage of phase composition of the samples has been estimated and values obtained are given in **Table -III.**

From the above crystallographic data , we can say that all four samples exhibit monoclinic phases as the dominant phase . It is also worth mentioning that in earlier studies ZrO2 doped with 12 mol% of Y2O3 were found to contain almost monoclinic phase (10).

Table - I

Sample codes and doped impurity

S.NO	Samples	Doped impurity	Stoichiometry of samples
1.	SZYP	P	$(ZrO_2)_{0.8}(Y_2O_3)_{0.2}$
2.	SZYTi	TiO_2	$(ZrO_2)_{0.8}(Y_2O_3)_{0.2}$
3.	SZYMn	$MnCl_2$	$(ZrO_2)_{0.8}(Y_2O_3)_{0.2}$
4.	SZYCu	$Cu(NO_3)_2$	$(ZrO_2)_{0.8}(Y_2O_3)_{0.2}$

Table -II

Crystallographic Data

hkl	Phases	d_{obs} A^0	d_{cal} A^0	$(d_{obs}-d_{cal})$ A^0	$(I/I_0)_{obs}$ %
[110],[011], [111]	M	3.60	3.64	0.04	24
[111]	M	3.12	3.16	0.04	77
[111]	T,C	3.02	2.97	0.05	100
[111]	M	2.80	2.84	0.04	76
[200],[002]	M,C	2.89	2.56	0.03	30
[210]	M	2.30	2.28	0.02	8
[102]	M	2.17	2.18	0.01	21
[112]	T	2.06	2.10	0.04	10
[112]	M	1.98	2.01	0.03	20
[002]	M	1.86	1.85	0.01	70
[202], [220], [220]	T,C,M	1.80	1.81	0.01	72
[002], [300]	M	1.68	1.96	0.01	16
[013]. [221]	M	1.64	1.64	0.00	38
[113], [311], [311] [131]	T,C,M	1.56	1.55	0.01	49
[222], [222], [311]	C,M	1.47	1.47	0.00	16
[132]	T	1.34	1.37	0.03	6
[104]	M	1.31	1.32	0.01	26
[400], [004]	C,T	1.29	1.28	0.01	16
[400]	C	1.26	1.26	0.00	16
--	-	1.22	1.23	0.01	10
[114]	T	1.21	1.21	0.00	20
[400]	T	1.10	1.10	0.00	11
[004]	T	1.09	1.09	0.00	9

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Table -III

Shows the relative phase composition

S.No	Samples Code	Relative Concentration of Phases (%)		
		M	T	C
1	SZYP	61	33	6
2	SZYTi	58	33	9
3	SZYMn	63	32	5
4	SZYCu	62	32	6

Fig. a & b

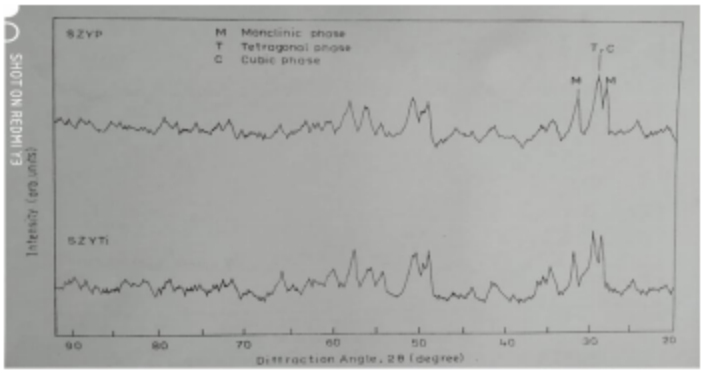
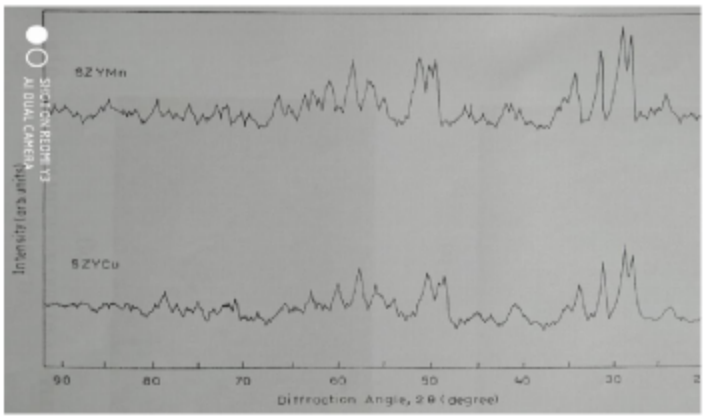


Fig. a & b



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