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LATTICE VARIATION AND MICROHARDNESS OF $NaCl_x$ $NaBr_{y-x}$ KCl_{1-y} MIXED CRYSTALS GROWN FROM AQUEOUS SOLUTION

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ABSTRACT

Mixed crystals of alkali halides find their application in optical, optoelectronics, and electronic devices. In the present study, ternary mixed crystals of $NaCl_x$ $NaBr_{y-x}$ KCl_{1-y} were grown from the aqueous solution. The grown crystals were characterized by taking XRD and Vicker's microhardness measurement. Lattice Parameters were determined from the X-Ray diffraction data by available method. The hardness number and work hardening coefficient were determined from the hardness value. The lattice parameter thus calculated obey Vegard's law and the work hardening coefficients shows that the grown crystals belong to hard category material

1 Introduction

The alkali halide crystals have importance in past six decades. They have been "model crystals" for testing many solid state theory. They are widely used as laser window materials ,neutron monochromators, infra red transmitters etc. But the users are limited by their mechanical properties and stability in some cases. Hence, their exists the need to strengthen them and improve the stability. Armington etal [1] discussed two methods of improving the hardness of alkali halides (i) solid solution hardening and (ii) impurity hardening.

A mixed crystal is obtained by crystallizing together two or more isomorpous crystals with comparable lattice constants. Alkali halide mixed crystals are of completely disordered substitutional type. Several reports are available on binary mixed crystals of alkali halides[2-4]. However limited reports are available on ternary and quartnery mixed crystals on microhardness. In the present study, ternary mixed crystals of $NaCl_x$ $NaBr_{y-x}$ KCl_{1-y} were grown by slow evaporation tecqnique and characterized them by X-ray diffraction and Vicker's micro hardness measurement.

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2.Experimental details

2.1.Growth of sample crystals

AnalaR grade NaCl,NaBr,and KCl, and doubly distilled water were used for the preparation of sample crystals. Supersaturated solutions of $NaCl_x$ $NaBr_{y-x}$ KCl_{1-y} were prepared for various values of x(0.2 to 0.7, in steps of 0.1) and y[0.6 and 0.8]. In the present study totally 10 (3 pure end member crystals and 7 mixed crystals) were grown in identical conditions. The end member crystals were grown for comparision purposes. The composition of the mixed crystals were estimated from the EDAX data for all the mixed crystals.

2.2.Lattice parameters

X-ray diffraction data were collected from powdered samples using an automated X-ray powder diffractometer with monochromated CuK_α (□□1.5406Å) radiation. The reflections were indexed following the procedure of Lipson and Steeple [5].

The lattice parameters were also calculated from the Vegard's law

$$a = xa_1 + (y-x)a_2 + (1-y)a_3$$

where a_1, a_2 and a_3 are lattice parameters of NaCl, NaBr and KCl respectively x and y are compositions.

2.3.Microhardness measurement

The hardness of a material is defined as [6] the resistance it offers to the motion of dislocations, deformation or damage under an applied stress. Hardness testing provides useful information on the strength and deformation characteristics of materials [7]. It is correlated with other mechanical properties like elastic constants [8] and yield stress [9]. Meyer [10] established a relationship between indentation hardness and plastic and work hardening capacity of a material.

Vicker's microhardness measurements were done on all the ten crystals grown using Zeitz Wetzler hardness tester fitted with a diamond pyramidal intender and attached with Zeitz incident light microscope.

Indentation test was done in air at room temperature. Different loads (25g.50g.and 100g) were used for indentation. Diagonal length 'd' of indented impressions obtained for various loads were measured. The average value of the diagonal lengths of the indentation marks in each trial was calculated. Hardness of the crystal was calculated using the relation,

$$H_v = 1.8544(P/d^2) \text{ kg/mm}^2$$

where P is applied load in kg and 'd' the average diagonal length in mm.

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To know hardness of the materials a graph of logP versus logd is plotted. The slope of the best linear fit gives Meyer's work hardening coefficient 'n'.

System	Estimated composition	Lattice Parameter	
		Observed	Vegard's law

3. Results and discussion

The crystals grown in the present study are shown in fig (i).The mixed crystals are found to be more hard, stable and transparent when compared to the end member crystals..

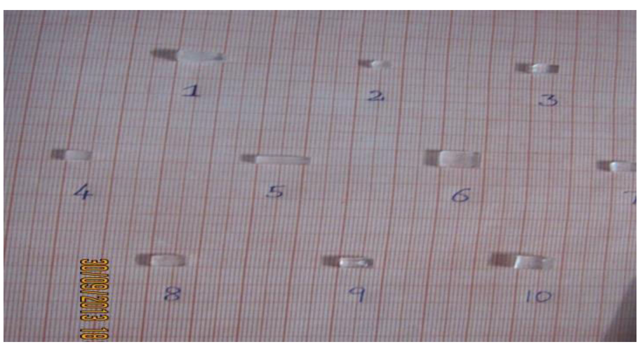

Figure 1 Photographs of grown crystal

The lattice parameters obtained in the present study along with those estimated from Vegard's law are provided in table 1.

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SYSTEM	HARDNESS VALUE				n VALUE
	25gm		50gm	100gm	
NaCl				5.6664	
NaBr				5.977	
KCl				6.3114	
$NaCl_{.2}$, $NaBr_{.4}KCl_{.4}$	0.169	0.441	0.390	6.4876	6.0858
$NaCl_{.3}$, $NaBr_{.3}KCl_{.4}$	0.330	0.307	0.362	5.6604	6.0672
$NaCl_{.5}$, $NaBr_{.1}KCl_{.4}$	0.504	0.107	0.392	5.67143	6.0787
$NaCl_{.4}$, $NaBr_{.4}KCl_{.2}$	0.39	0.402	0.189	5.6714	6.0290
$NaCl_{.5}$, $NaBr_{.3}KCl_{.2}$	0.489	0.304	0.191	5.6582	6.0144
$NaCl_{.6}$, $NaBr_{.2}KCl_{.2}$	0.537	0.189	0.232	5.6465	6.0335
$NaCl_{.7}$, $NaBr_{.1}KCl_{.2}$	0.607	0.107	0.188	5.6513	6.0344

According to Tobolsky [8] two alkali halides AB and AC will form continuous solid solutions AB_xC_{1-x} at 20°C, provide difference δ between their lattice parameters is less than 6%. Two compounds or elements are said to form a continuous solid solution if a single lattice parameter as measured by X-ray powder photographs can be assigned to the solid solutions at all compositions. In the present study, from the table1, it is found that all the ternary mixed crystals of the $NaCl_x$ $NaBr_{y-x}$ KCl_{1-y} are assigned single lattice parameter and it indicates that they form a continuous solid solution.

The microhardness value and the work hardening coefficient for all the grown crystals are provided in table2.

Table2: Micro hardness value and work-hardening co-efficient

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NaCl	20.5	25.5	45.15	0.2091
NaBr	21.25	27.35	33.15	0.2430
KCl	16.35	23.15	36.15	0.1853
$NaCl_{.2}$, $NaBr_{.4}KCl_{.4}$	13.15	18.5	36.25	0.1615
$NaCl_{.3}$, $NaBr_{.3}KCl_{.4}$	15.4	22.6	38.1	0.1803
$NaCl_{.5}$, $NaBr_{.1}KCl_{.4}$	23.4	27.25	39.45	0.3108
$NaCl_{.4}$, $NaBr_{.4}KCl_{.2}$	11.8	17.6	25.75	0.2213
$NaCl_{.5}$, $NaBr_{.3}KCl_{.2}$	13.2	21.25	36.5	0.1363
$NaCl_{.6}$, $NaBr_{.2}KCl_{.2}$	11.7	17.95	29.25	0.1464
$NaCl_{.7}$, $NaBr_{.1}KCl_{.2}$	12.15	25.45	37.25	0.1709

It is observed that hardness values for intermediate compositions are greater than the end member crystals and for higher and lower concentrations of NaCl, it is found to be less than the end member crystals. Also it varies non-linearly with bulk composition. Surdeshmukh [11]and Srinivas pointed out in their review paper that the replacement of ion by another ion of different size(size effect). In mixed crystals, results in a highly non linear composition variation in properties like the Debye-Waller factor, the dislocation density and hardness Subbarao [12] and HariBabu pointed out that in a mixed crystal, lattice interaction as well as the disorder due to size effect contribute to the hardness. On the other-hand, Srivatsava [13] considered the effect of the presence of substituted ions on the dislocation mobility and on the hardness.

A graph between logP and logd is shown in fig2.

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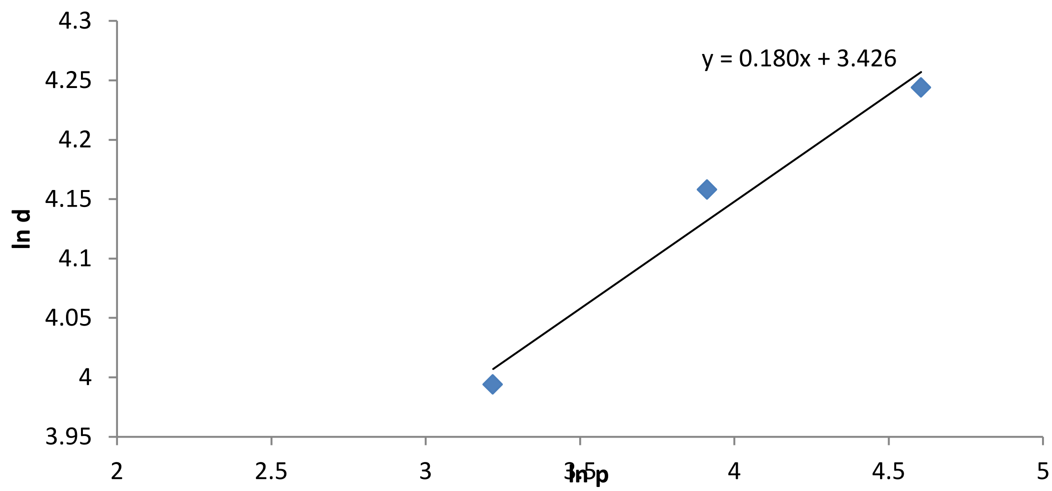

Fig 2 Variation of logP and logd for $NaCl_{.3}$,$NaBr_{.3}$,$KCl_{.4}$

The slope of the best linear fit of the above graph is Mayer's work hardening coefficient ,"n", the n values for the different compositions are provided in table2.According to Onitsch [14] and Hanneman [15] the 'n' value falls below 1.6 for hard materials and more than 1.6 for soft materials. The values obtained in the present study imply that the mixed crystals belong to hard material category.

4 Conclusion

The lattice parameter determined shows that the mixed crystals form a continuous series. The hardness numbers shows that the mixed crystals are harder than the end member crystals. The work hardening co-efficient determined in the present study implied that the crystals belong to hard category materials.

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