Bulk Modulus and Compressibility of $Nacl_xnabr_{(Y-X)}Kcl_{(1-Y)}$ Ternary Mixed Crystals Grown from Aqueous Solutions

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***Abstract*-Alkali halide crystals were found to be more useful in their applications ranging from monochromators to tunable lasers .In the present study ternary mixed crystals of $NaCl_xNaBr_{(y-x)}KCl_{(1-y)}$ were grown by slow evaporation technique. The grown crystals were characterized by taking XRD and Vicker's micro-hardness measurement. The bulk modulus and compressibility were determined from the Debye temperature which is calculated from the Debye Waller factor and hardness number both compressibility values agreed with each other.**

I. INTRODUCTION

A vast amount of information has been generated with regard to all aspects of alkali halide crystals over several decades due to their importance as model crystals and their potential as device material. A mixed crystal, in general has physical properties analog as to those of the end member crystals.

The composition dependence varies from system to system and property to property. The property changes in many cases monotonically with composition in a linear or nearly linear manner. Several reports are available on binary mixed crystals of alkali halides [1-3].Mixed and impurity added crystals of alkali halides are found to be harder than the end member crystals and hence the application visibility of alkali halides are enhanced and improved.

Sirdeshmukh et.al [1] reported that impurity hardening is more effective than solid solution hardening. So in the present study we grow the pure and ternary mixed crystals of NaCl, NaBr and KCl.

II. EXPERIMENTAL DETAILS

2.1.Growth of sample crystals

Analytical Reagent (AR) grade NaCl, NaBr and KCl substances and doubly distilled water were used in the present investigation. An aqueous solution of the salt with desired molecular ratio was prepared at supersaturated concentration. The temperature and volume were kept constant respectively at 32^{o}C and 100ml for all the crystals. In the present study total of ten crystals (three end members seven mixed crystals) for various values of x and y were grown in identical conditions.

2.2.Estimation of bulk composition

The compositions of pure and mixed crystals were accurately estimated from EDAX spectrum taken by SUTW- SAPPIRE DIRECTOR OF 1339.91 RESOLUTION.

2.3 Bulk modulus and compressibility

The compressibility (Ψ) of all the grown crystals were determined from the Debye Waller factor (reported elsewhere[4]) using the formula [5]

$$\Theta_D = A\Psi^{(1/2)}M^{(-1/2)}V^{(1/6)}$$

Where A is a constant. Here it is $1.176*10^{12}$ and Ψ is the compressibility, M is the molecular weight of the crystal and V is the volume of the crystal.

The Vickers microhardness were determined from the Zeitz Wetzler hardness test filled with a diamond pyramidal intender and attached with Zeitz incident light microscope. Intentation test was done in air at room temperature different loads (25 gm,50 gm and 100gm) where used for intentation multiplication of hardness number with $9.8*10^{-3}$ gives the bulk modulus of the crystals in GPa. The reciprocal of the bulk modulus K gives the compressibility.

2.4 Results and Discussions

The crystals grown in the present study are stable,transparent and good quality. All the crystals grown in the present study are shown in the figure 1 .

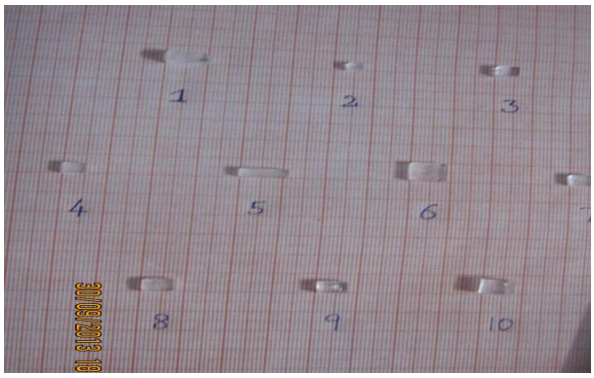

Figure 1.Photograph of sample crystals.

The compressibility and bulk modulus is given in table 1 and table 2.

Table 1 Compressibility from Debye Waller factor

system	Molecular weight(gm)	Lattice constant a (A°)	Debye value factor Θ_D (k)	Compressibility Ψ (10^{-12} m^2/Newton)
NaCl	58.44	5.66	275 (278)	5.668 (5.668)
NaBr	102.9	5.977	202 (202)	4.888 (5.02)
KCl	74.54	6.30	196.6 (206)	3.178 (5.73)
$NaCl._2$, $NaBr._4KCl._4$	62.97	6.292	148.77	1.585
$NaCl._3$, $NaBr._3KCl._4$	68.57	5.769	170.15	2.393
$NaCl._5$, $NaBr._1KCl._4$	68.6	5.827	188.03	2.783
$NaCl._4$, $NaBr._4KCl._2$	55.17	5.852	126.94	1.056
$NaCl._5$, $NaBr._3KCl._2$	61.42	5.843	245.25	4.426
$NaCl._6$, $NaBr._2KCl._2$	56.03	5.943	229.31	3.446
$NaCl._7$, $NaBr._1KCl._2$	50.09	5.744	248.08	6.724

Table 2 Compressibility from Vickers hardness measurement

system	H_v 100 gm	Bulk modulus K (GPa)	Compressibility Ψ=(1/K)
NaCl	45.15	.4424	2.260
NaBr	33.15	.3248	3.078
KCl	36.15	.3542	2.823
$NaCl._2$, $NaBr._4KCl._4$	36.25	.3552	2.815
$NaCl._3$, $NaBr._3KCl._4$	38.1	.3733	2.678
$NaCl._5$, $NaBr._1KCl._4$	39.45	.3866	2.5866
$NaCl._4$, $NaBr._4KCl._2$	25.75	.2523	3.963
$NaCl._5$, $NaBr._3KCl._2$	36.5	.3577	2.780
$NaCl._6$, $NaBr._2KCl._2$	29.25	.2866	3.489
$NaCl._7$, $NaBr._1KCl._2$	37.35	.3660	2.732

The compressibility determined for the end member crystal well agreed with both the cases and the compressibility determined for the mixed crystals by Vickers hardness measurement agreed with the compressibility values determined from the Debye value factor.

CONCLUSION

The compressibility of all the grown crystals determined from Debye temperature and Vickers hardness number agreed with each other and agreed with the reported values for end member crystals.

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