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X-RAY Characterization of Mixed KCl_xBr_{1-x} Crystals

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Abstract: *The present chapter is on X-ray characterization of mixed KCl_xBr_{1-x} single crystals. The distance 'd' between adjacent (100) planes has been found to vary in a linear way with the change of x for different KCl_xBr_{1-x} crystals, studied through X-ray diffraction analysis.*
Keywords: *X-ray, KCl_xBr_{1-x} crystals, diffraction*

I. Introduction

The X-ray diffraction characterization helps to as certain formation of any new compound in a solid state reaction. The alkali halide crystals have always been at the center state of solid-state physics.The use of pure simple alkali halides is limited by the mechanical systems and hence there exist the need to strengthen them. The mixed and impurity added (doped) crystals of alkali halides are found to be harder than the end members and so they become more useful in these applications [1]. X-ray diffraction analysis indicates that the salts are bound in the solid state as contact ion pairs. Haribabu and Subbarao[2]have reviewed the aspects of the growth and characterization of alkali halide mixed crystals. Sirdeshmukh and Srinivas[3] have reviewed the physical properties. Mahadevan and his co-workers [4] obtained largerand more stable crystals from $(NaCl)_x(KCl)_{0.9-x}(KBr)_{0.1}$ solutions than from $Na_xK_{1-x}Cl$ solutions.S.Perumal*et al*.[5] have reported the Growth and characterization of multiphased mixed crystals of KCl, KBr and KI:1.,Accordingly, the growth and characterization of mixed KCl_xBr_{1-x} single crystals, used for study in this work are presented, as in the following.

II. Growth of crystals

It was thought appropriate to grow single crystals of KCl_xBr_{1-x} system by the saturated solution method [6]. Accordingly, the appropriate mass ratios of KCl and KBr were dissolved in distilled water to yield a saturated solution. The resulting solution was left for slow evaporation for a couple of days, when small sized (3mm *x* 3mm *x*2mm) crystals appeared for each of the five values of *x* as 0.0, 0.7, 0.8, 0.9 and 1.0 proposed in this work. The crystals were taken out from water solution, dried and kept for X-ray characterization and other measurements.

III. X-ray Characterization

In order to establish that KCl and KBr mix properly and yield only a cubic phase, X-ray diffraction (XRD) characterization was done of KCl_xBr_{1-x} samples for x = 0.0, 0.7, 0.8, 0.9 and 1.0.The XRD – patterns were recorded for the powder samples using a X-ray diffractometer, model Iso – Debyeflex 2002, having a Cu K_α source with the current setting at 20 mA and voltage across the cathode & target being 30 kV.

Figs. 1.1 to 1.5 give the XRD patterns for the five samples as above. Tables 1.1 & 1.2 give the diffracted X-ray intensity vs. angle (2θ) data for these samples. The XRD patterns show 100% intensity for reflections from (100) planes. Further, it is seen that the d-separation between two adjacent (100) planes [7] shows a regular variation with the continuous addition of KCl to KBr.

Table 1.1 XRD intensity for different 2θ peaks for pure crystals

for pure KBr			for pure KCl		
Intensity %	**Angle in degrees (2θ)**	**d(A°)**	**Intensity%**	**Angle in degrees (2θ)**	**d(A°)**
25.40	23.54	3.779	100.00	28.46	3.136
100.00	27.03	3.299	8.18	31.96	2.800
99.60	38.44	2.341	54.28	40.62	2.221
18.70	45.42	1.997	11.05	50.13	1.819
26.32	47.56	1.911	13.22	58.63	1.574
31.31	55.53	1.654	27.74	66.39	1.408
11.35	60.96	1.519	12.62	73.79	1.284
43.16	63.81	1.479			
23.73	69.68	1.379			

The graph of Fig. 1.6 shows variation of 'd(100)' parameter for KCl_xBr_{1-x}, when x is varied as 0.0, 0.7, 0.8, 0.9 and 1.0. The graph obtained is almost linear, indicating good miscibility of KCl in KBr, leading to the formation of mixed cubic lattices. The graph further shows the change of lattice size in a regular fashion with the variation of x.

Table 1.2 XRD intensity for different 2θ peaks for mixed crystals

for $KCl_{0.7}$ $Br_{0.3}$			for $KCl_{0.8}$ $Br_{0.2}$			for $KCl_{0.9}$ $Br_{0.1}$		
Intensity %	**Angle in degrees (2θ)**	**d(A°)**	**Intensity %**	**Angle in degrees (2θ)**	**d(A°)**	**Intensity %**	**Angle in degrees (2θ)**	**d(A°)**
100.0	28.08	3.178	100.00	28.21	3.163	100.00	28.27	3.156
66.35	40.12	2.247	41.58	40.25	2.240	34.44	40.44	2.230
17.24	49.68	1.835	15.45	49.89	1.828	10.11	49.99	1.824
13.94	58.01	1.589	12.36	58.34	1.581	13.16	58.36	1.581
24.79	65.74	1.420	21.28	66.20	1.411	10.98	66.04	1.414
10.85	72.92	1.297	15.46	73.58	1.287	07.77	73.28	1.291

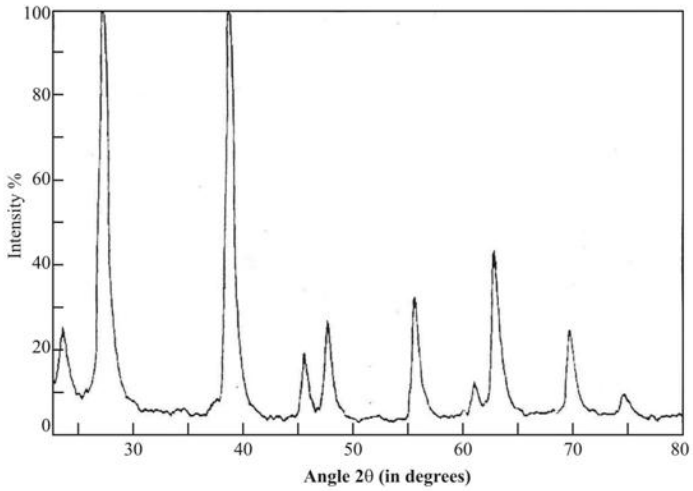

Fig.1.1 XRD Intensity for different 2θ peaks for pure KBr

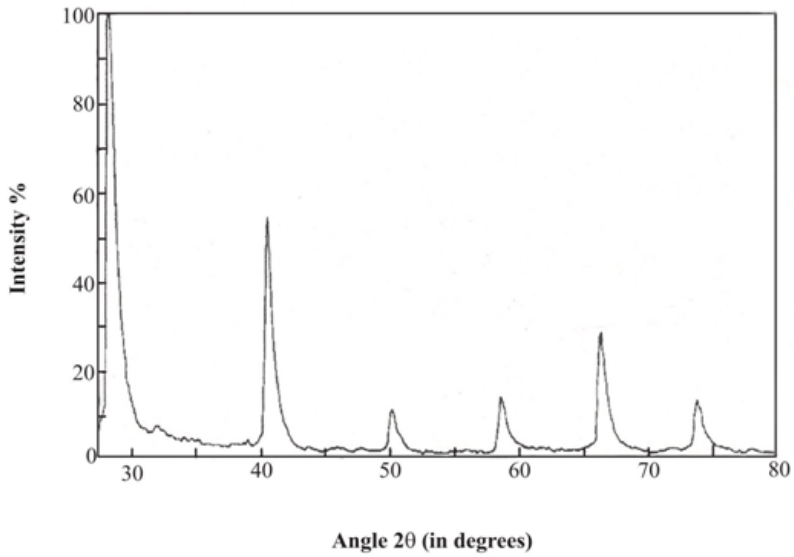

Fig.1.2 XRD Intensity for different 2θ peaks for pure KCl

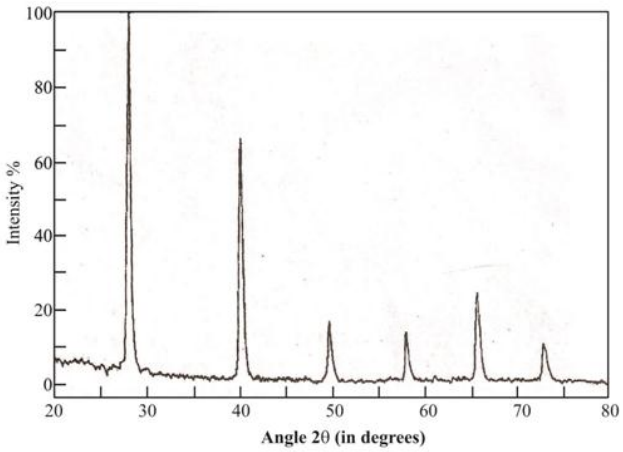

Fig.1.3 XRD Intensity for different 2θ peaks for pure $KCl_{0.7}Br_{0.3}$

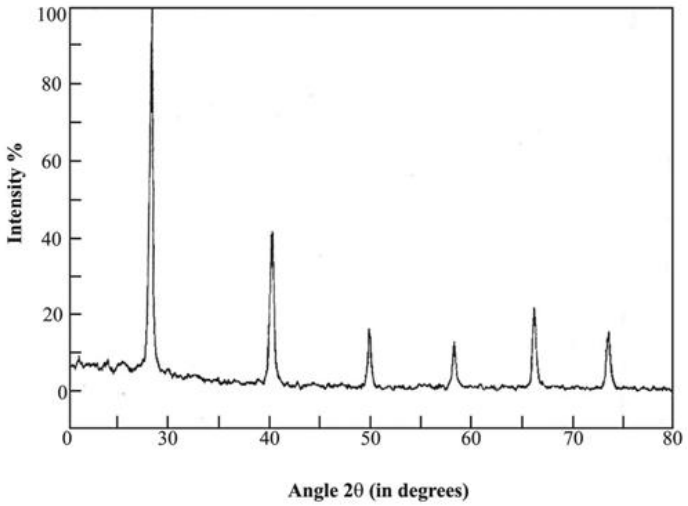

Fig.1.4 XRD Intensity for different 2θ peaks for pure $KCl_{0.8}Br_{0.2}$

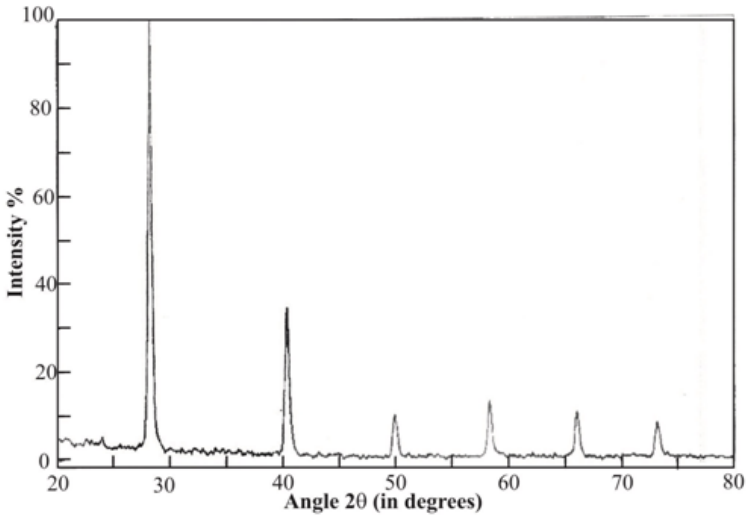

Fig.1.5 XRD Intensity for different 2θ peaks for pure $KCl_{0.9}Br_{0.1}$

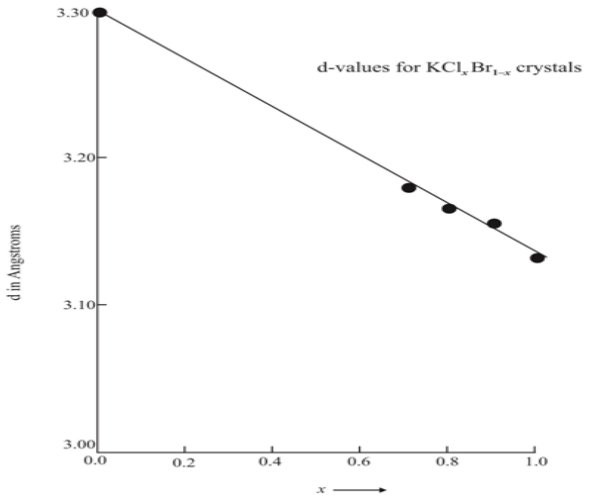

Fig.1.6 variation of d-parameter for KCl_xBr_{1-x}

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