



## A STUDY OF TERNARY MIXED ALKALI HALIDE CRYSTALS GROWN BY AQUEOUS SOLUTION METHOD

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### ABSTRACT:

A slow-evaporation method used to produce single ternary mixed alkaline  $(KCl)_x(KBr)_{0.9-x}(NaI)_{0.1}$  crystals from various compositions. Under similar circumstances all crystals were grown. The obtained crystals were tested using XRD. In order to know the elementary analysis, EDAX data have been obtained for the samples. The Zwick hardness test with a Vicker diamond pyramid indenter was used for microhardness measurements. Dielectric constant and dielectric loss measurement was performed using the 1kHz to 10 MHz LCR metre. The development of a ternary mixed crystal is seen to be associated with increased hardness and changes with composition in a nonlinear way. The elastic rigidity constant (C11) of crystals was calculated for different loads using the hardness measurement.

**KEYWORDS:** Ternary, Mixed Alkali Halide, Crystals, Aqueous, Elastic stiffness constant.

### INTRODUCTION:

Alkali halide mixed crystals are widely utilised as Laser Fensters, Neutron monochromers, Infrarot Transmitters, etc. But the usage of simple alkali halides is restricted and strengthened by mechanical systems. The mixed crystals of the alkaline halides added to them and are impurities more difficult to utilise than the ending members. It is also recognised that alloys in device manufacturing are better than pure plain metals. In this respect, the preparation and the investigation of their physical characteristics of binary and ternary mixed crystals without consideration for miscibility issues is required and beneficial. In the current study effort, a sluggish slow evaporation method is used to produce single glasses of ternary mixed alkali halides  $(KCl)_x (KBr)_{0.9-x}(NaI)_{0.1}$  with investigations of microhardness and dielectric constant.

### METHODOLOGY

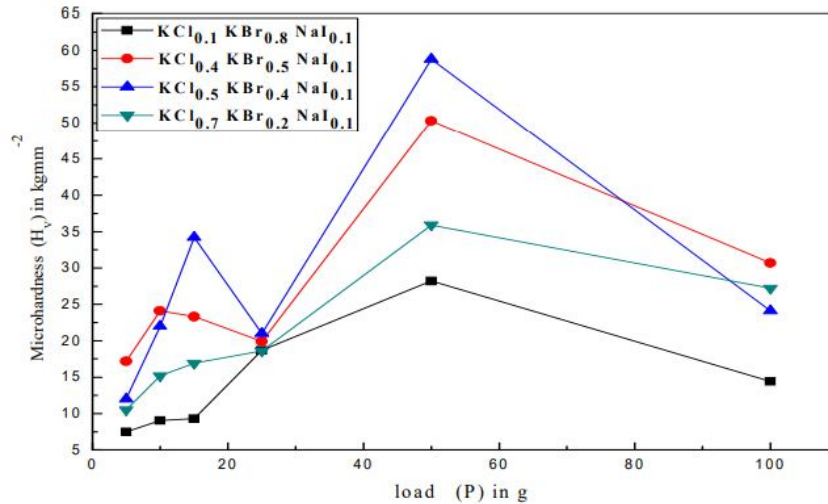
The slow evaporating approach used by an analogue grade of KCl, KBr and NaI as starting ingredients for the development of the crystals produced the Ternary  $(KCl)_x(KBr)_{0.9-x}(NaI)_{0.1}$  mixed crystals. Clear translucent crystals have been obtained well defined. All crystals have been cultivated under the same circumstances.

Grown crystals had been sliced and constantly measured using micro-hardship and dielectricity.

**RESULTS AND DISCUSSION**

**Microhardness studies**

The Zwick 3212 hardness tester with a Diamond Pyramidal Indenter from Vicker has been used for micro hardness measurements. On the newly closed samples all indentation measurements were performed. The load was loaded from 5 to 100 grammes, and the indentation time was maintained at 10 seconds. The imprints were about quadratic. At several locations the crystal surfaces were damaged. A calibrated micrometre connected to the microscope lens measured diagonal lengths in the indented prints Each sample was subjected to many indentations. In the calculation of hardness, the average value of the diagonal lengths of the mark was utilised.



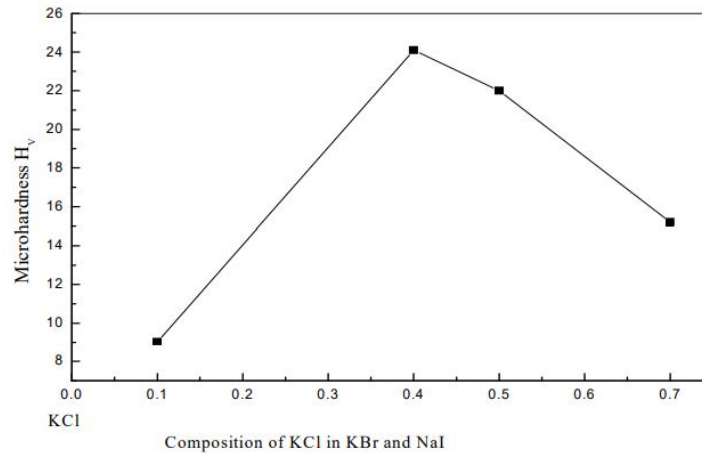
**Fig.1 Variation of microhardness with load**

The microhardness is calculated by the term [1].

$$H_v = 1.8544P/d^2 \text{ Kg mm}^{-2}$$

where P is the force applied to Kg and d is the average Vickers' diagonal length printing to mm following loading.

The development of gemixed crystals has been discovered to be associated by an increase in hardness and fluctuates in a nonlinear manner. Even if the hardness has been described in many ways, the resistance to dislocation movement is universally recognised presently. Some contributions to the dislocation resistance are made and may be divided into two categories (i) the intrinsic resistance dependent on a certain crystal-insensitive structure physical parameter, and (ii) the disorder parameter dependent on its imperfection concentration.



**Fig.2 Variation of microhardness with composition**

The non-linear fluctuation in composition of the micro-hardness is attributable to defects. These defects might be vacancies, unclean-vacancy pairs, dislocations etc. Research reveals that mixed-crystal conductivity is high for mixed-glasses compared to the end-crystals. The conductivity of mixed-crystals is high. Since ionic conductivity is attributable entirely to charged vacancies, these results thus show that these vacancies are concentrated. The result on dislocation morphology [3] demonstrates that mixed crystal has more low-angle kernel bordings and dislocations than pure crystals. The formation of low angle grain boundaries in mixed crystal might also be attributable to Tiller's eutectic crystallisation mechanism [4]. Vacancies, dislocations and grain borders therefore seem to be the major defects in blended crystals, and this might lead to the observed nonlinear fluctuation of the micro-hardness inherent.

**Table.1 Pauling ionic radii IN Å**

Ion	Ionic size Å
$\text{Cl}^-$	1.81
$\text{Br}^-$	1.95
$\text{I}^-$	2.16
$\text{K}^+$	1.33
$\text{Na}^+$	0.95

Lattice strains are common to everyone owing to the variation in atom size or ions in mixed crystals.

The size of different ions [5] is shown in table.1.

A chart of  $\log P$  against  $\log d$  is drawn to determine the hardness of the materials. Mayers work hardening coefficient 'n' comes from the pendulum of the best linear fit graph. Table shows the n values for various compositions. 2. The 'n' value falls under 1.6 in hard materials and more than 1.6 in soft materials, according to Onitsch [6] and Hanneman [7]. The values achieved suggest that the mixed crystals are categorised as hard materials.

Table.2 Work hardening co-efficient

Composition	'n' Value
KCl <sub>0.1</sub> KBr <sub>0.8</sub> NaI <sub>0.1</sub>	0.33
KCl <sub>0.4</sub> KBr <sub>0.5</sub> NaI <sub>0.1</sub>	0.38
KCl <sub>0.5</sub> KBr <sub>0.4</sub> NaI <sub>0.1</sub>	0.36
KCl <sub>0.7</sub> KBr <sub>0.2</sub> NaI <sub>0.1</sub>	0.32

Table.3 Values of Elastic stiffness constant

Load (p) in g	C <sub>11</sub> for KCl <sub>0.1</sub> KBr <sub>0.8</sub> NaI <sub>0.1</sub> (×10 <sup>14</sup> Pa)	C <sub>11</sub> for KCl <sub>0.4</sub> KBr <sub>0.5</sub> NaI <sub>0.1</sub> (×10 <sup>14</sup> Pa)	C <sub>11</sub> for KCl <sub>0.5</sub> KBr <sub>0.4</sub> NaI <sub>0.1</sub> (×10 <sup>14</sup> Pa)	C <sub>11</sub> for KCl <sub>0.7</sub> KBr <sub>0.2</sub> NaI <sub>0.1</sub> (×10 <sup>14</sup> Pa)
5	33.8	145.3	77.4	61.2
10	47.0	262.1	223.5	117.0
15	49.4	247.1	483.7	140.8
25	168.0	187.5	206.0	166.6
50	345.1	950.0	1248.0	526.5
100	106.4	400.0	262.0	324.0

The elasticity constant (C<sub>11</sub>) has been calculated using Wooster's empirical method  $C_{11} = H^{7/4}$  for different compositions as well as for varied loads. Table.3 displays the values of C<sub>11</sub>. These numbers provide an insight into the tightness of adjacent atoms [8]. Among the combinations tested, atoms in the sample KCl<sub>0.5</sub> KBr<sub>0.4</sub> NaI<sub>0.1</sub> are more closely linked to their nearby atoms.

The sample KCl<sub>0.5</sub> KBr<sub>0.4</sub> NaI<sub>0.1</sub> replies for a higher value of C<sub>11</sub> for all loads between 5gm and 50gm among the samples studied.

#### Dielectric studies and a.c. Conductivity (σ<sub>ac</sub>)

The samples were ground and polished to the right thickness. The samples were finally 1.5 to 2 sq.cm in area, with a thickness of 0.1 to 0.3 cm. The air-dry silver-paste of each specimen was electroded to act as a parallel plate-condenser on both sides. A sample capacitance (C) and dissipation factor (D) were measured with a 4275A multi-frequency LCR (Hewlett-Packard) metre as a requirement offset function. The dielectric constants, dielectric losses and ac conductivity from C to D have been computed using the relationships,

$$\epsilon_r = Cd / \epsilon_0 A, \tan \delta = D \epsilon_r \quad \text{and} \quad \sigma_{ac} = \epsilon_0 \epsilon_r \omega \tan \delta$$

#### Glossary of symbols

C – Capacitance of a capacitor d – Plate separation

A – Area of plate

D – Dissipation factor

ω -- Angular frequency

ε<sub>r</sub> – Dielectric Constant

ε<sub>0</sub> - Permittivity of free space.

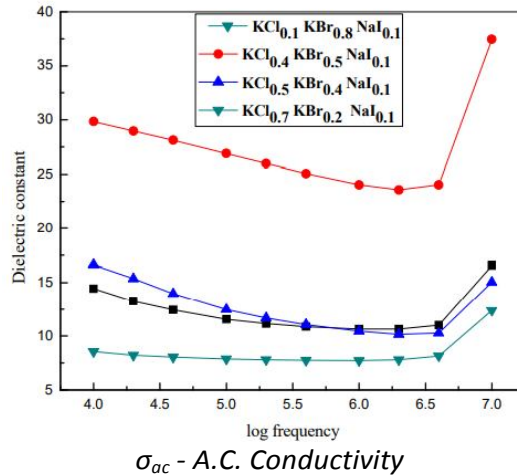


Fig.3 Variation of dielectric constant ( $\epsilon_r$ ) with frequency

Figure 4 shows the fluctuation of  $\sigma_{ac}$  and frequency.

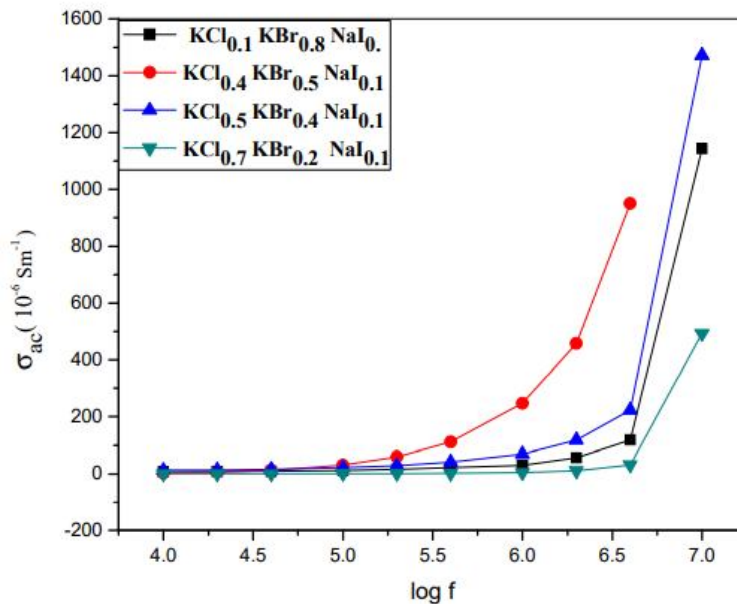


Fig.4 variation of AC conductivity with frequency

The fluctuation of  $\sigma_{ac}$  and frequency is virtually consistent up to 100 KHz for all the samples examined. Subsequently, in keeping with stated results, the exponential fluctuation with frequency showed [9].

### CONCLUSIONS

A slow evaporation from the aqueous solution resulted in good optically clear ternary mixed alkaline halide crystals  $(KCl)_x(KBr)_{0.9-x}(NaI)_{0.1}$  of various compositions. Elemental analysis EDAX verified. Nonlinear composition of microhardness has changed. In ternary mixed crystals, microhardness is greater than in pure binary mixed crystals. The increase in the hardness of combined crystals is due to the internal stresses resulting from the difference in ionic dimensions, which causes the production of

dislocations, grain borders with low angles and other defects. Of the combinations under investigation, atoms in  $KCl_{0.5}KBr_{0.4}NaI_{0.1}$  are closely connected with their nearby atoms.

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