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Comparative study of dielectric properties of Ternary Alkali Halide crystals

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Abstract : Crystals, especially alkali halides are the ideal ones for theoretical as well as experimental research. In modern day technology, crystal growth research has been the important subject in materials science and condensed matter physics, because of their importance in the modern devices. Present work deals with growth of alkali halide single crystals of various compositions containing KCl, KBr, NaCl, NaBr and NaI. Two sets of ternary crystals were grown using these alkali halides. A comparative study of dielectric studies and A.C. conductivity as a function of frequency has been carried out for both the sets of crystals.

Key words : Ternary crystals, Dielectric constant, A.C. Conductivity.

1. Introduction

Alkali halides are the convenient systems for scaling of properties. The lattice constant has been used to scale a large number of properties like elastic constants, hardness, colour centre parameters like concentration of defects, Debye's temperature, etc.

Thus, whether it was testing of theories or trying new experiments, the alkali halides have always played a leading role as model crystals. In 1946 Seitz remarked "In the field of material science, alkali halides are the most interesting crystals as they have continuously yielded to persistent investigation and have gradually provided better and better understanding of the most interesting properties of all solids". The statement remains relevant even today (1). In the last few decades the alkali halides emerged as crystals with useful applications. The polycrystalline alkali halides are used as laser window materials (2, 3). KCl-KBr mixed crystals have been employed as neutron monochromators, whereas LiF and NaCl are used as X-ray monochromators (4, 5). Several alkali halides are used in energy detection in the X-ray, γ -ray and Cerenkov regions. The alkali halide crystals have useful transmission properties in different ranges of the spectrum from UV to IR. While LiF, NaF and NaCl are useful in UV transmission, potassium bromide, potassium iodide, Caesium bromide and Caesium iodide are useful in IR transmission.

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2. Crystal Growth

Single crystals are grown by slow evaporation method. The ideal conditions for the growth of crystals is the temperature stabilization of $\pm 0.005^\circ\text{C}$ and rate of evaporation of few ml /hr. The major advantage of this technique is the crystals are grown at a fixed temperature. If the material has a low coefficient of temperature stability, then this is the suitable method for growing the crystals. This method demands the proper temperature control for the good growth rate of crystals.

Table.1 Dielectric constant (ϵ_r)values for various combinations

Dielectric constant (ϵ_r)values ata frequency of 1 MHz			
$\text{KCl}_{0.2}\text{NaCl}_{0.1}\text{NaBr}_{0.7}$	$\text{KCl}_{0.2}\text{NaCl}_{0.2}\text{NaBr}_{0.6}$	$\text{KCl}_{0.2}\text{NaCl}_{0.5}\text{NaBr}_{0.3}$	$\text{KCl}_{0.2}\text{NaCl}_{0.6}\text{NaBr}_{0.2}$
4.06	9.98	45.13	7.52
$\text{KCl}_{0.1}\text{KBr}_{0.8}$ $\text{NaI}_{0.1}$	$\text{KCl}_{0.4}\text{KBr}_{0.5}$ $\text{NaI}_{0.1}$	$\text{KCl}_{0.5}\text{KBr}_{0.4}$ $\text{NaI}_{0.1}$	$\text{KCl}_{0.7}\text{KBr}_{0.2}$ $\text{NaI}_{0.1}$
10.66	24.03	10.44	7.74

Alkali halides of comparable lattice constants are chosen to grow ternary mixed crystals. Complete miscibility for ionic compounds such as alkali halides will take place only if their temperature is above a certain critical value, T . This critical temperature is given by $T = 4.5 S^2$ where S is percentage difference in lattice constants. To satisfy this condition, we selected KCl, NaCl and NaBr alkali halides. Ternary crystals of $(\text{KCl})_x(\text{NaCl})_{y-x}(\text{NaBr})_{1-y}$ were grown for various values of x and y by slow evaporation technique. In a span of four to five weeks we obtained single crystals of reasonably good size for characterization. The EDAX analysis has shown the presence of all the three alkali halides in the grown mixed crystals.



KClNaClNaBr crystal



KClKBrNaI crystal

Experimental

The extended portions of the crystals were removed completely and the samples were ground to proper thickness and polished. the final dimensions of the samples were about 1.5 to 2 sqcm and 0.1 to 0.3 cm in thickness. Each sample was electroded on either side with air-drying silver paste so that it behaved like a parallel plate capacitor. a 4275a, multi frequency lcr meter (hewlett-packard) was used to measure capacitance (c) and dissipation factor (d) of the sample as a function of frequency. the dielectric constant (ϵ_r) was calculated from c and d using the relation,

$$\epsilon_r = \frac{Cd}{A\epsilon_0}$$

where,

C is the capacitance of the sample

D is the thickness of the sample

A area of the face in contact with the electrode and ϵ_0 the permittivity of free space.

3. Results and Discussion

The variation of dielectric constant(ϵ_r) with frequency at room temperature are shown in fig.1 and 2. The dielectric constant for both the combinations is found to become maximum for a particular combination of ternary mixed crystals. This shows that dielectric properties are modified with the mixing of crystals. Though dielectric constant decreases with increase in frequency due to inability of the molecules to cope up with changed direction of electric field, the sudden jump in the dielectric constant at 1 MHz is yet to be understood. The phenomena involved in the boosting of dielectric properties are to be studied.

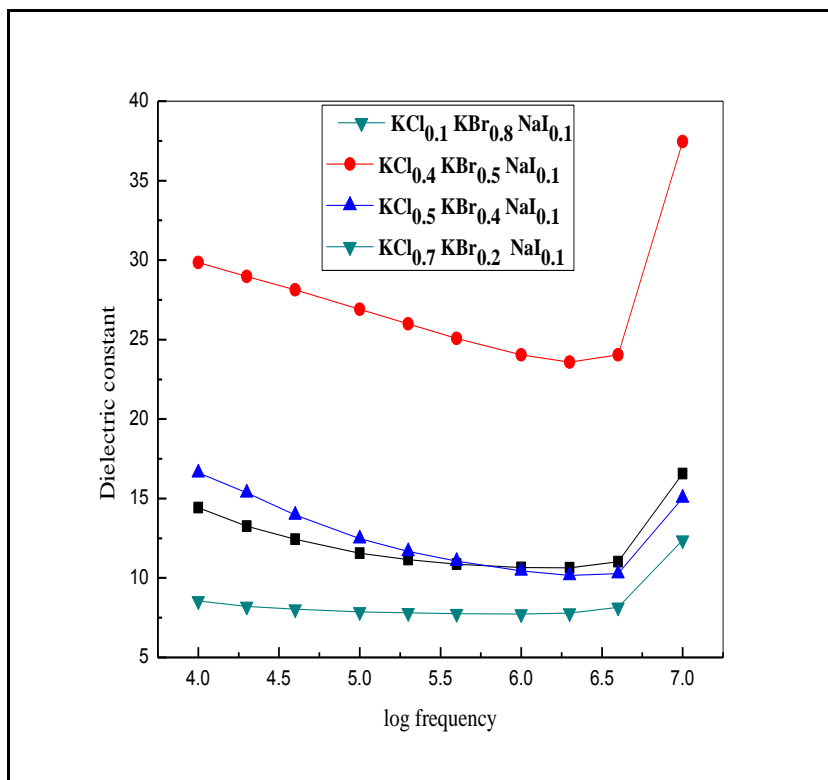


Fig.1

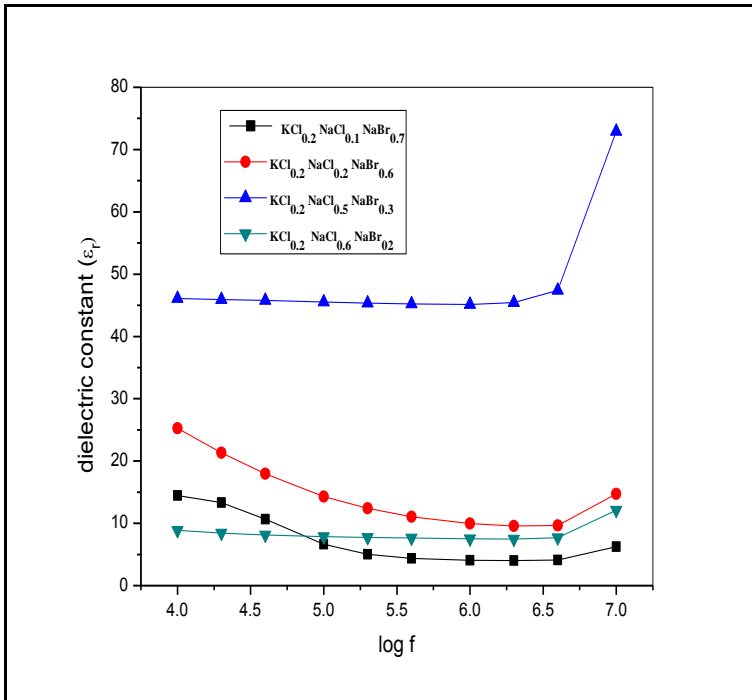


Fig. 2

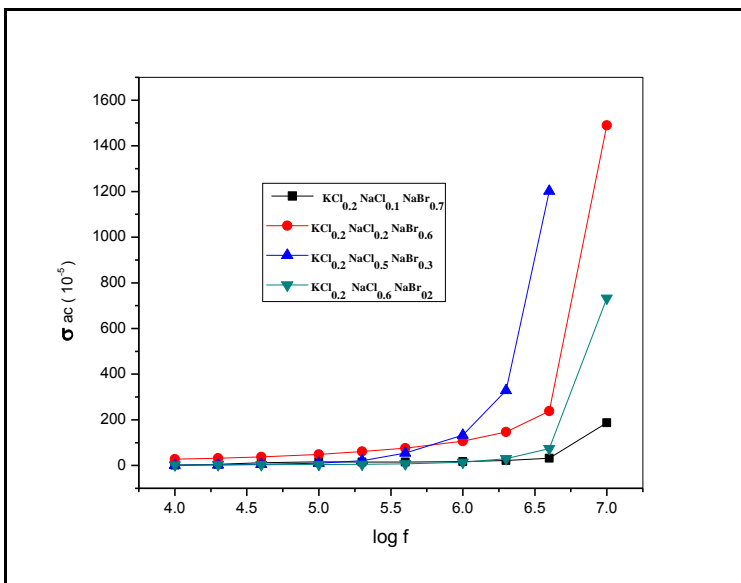


Fig. 3

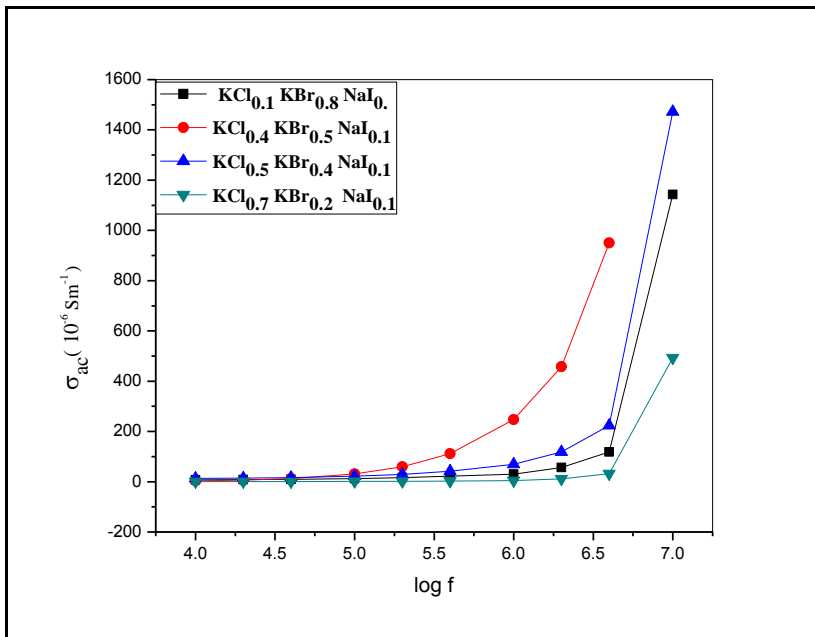
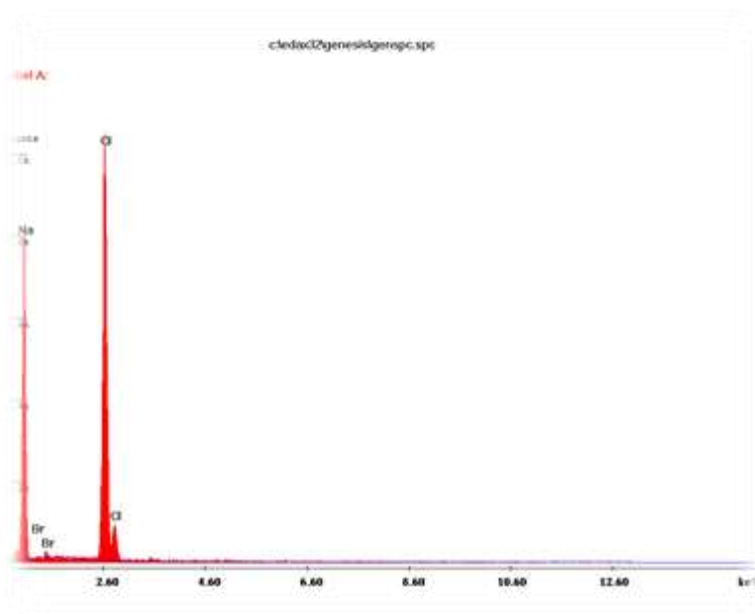
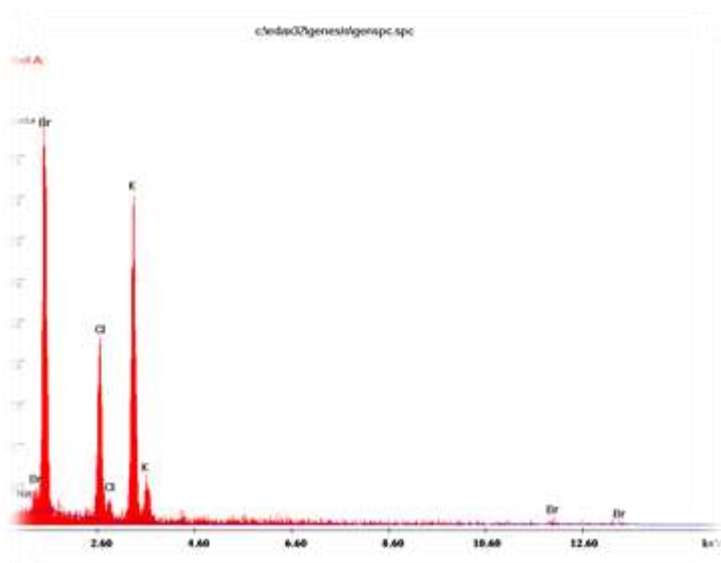


Fig.4





EDAX data of grown ternary alkali halide crystals

Conclusions

The A.C. conductivity of both the combinations are varying in expected manner but the rapid increment in the conductivity at high frequency is due to sudden jump in the dielectric constant value. Among various compositions investigated, many are suitable for making capacitors.

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