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Optical properties of $Na_xK_{1-x}Br$ crystals grown from aqueous solution

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ABSTRACT

Mixed crystals of alkali halides find their applications in optical, opto electronics and electronic devices. Binary mixed crystals of NaBr and KBr were grown by the slow evaporation method. Refractive indices of all the grown crystals were calculated using Abbe's refractometer and optical properties were determined by UV-Vis spectrometer. The detailed results are reported in this paper

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I. INTRODUCTION

Alkali halide crystals has always been at the center state of solid state physics and have proved useful in several applications ranging from X-ray monochromators to tunable lasers. The development of lasers revived the interest in alkali halides as materials for optical compositions. This led to the development of alkali halide polycrystalline materials for use as optical windows [1]. Several recent reports are also available on alkali halide crystals [2-5]

Alkali halides have large band gaps and so single crystals of alkali halides are transparent over a wide range of frequencies including visible, near infrared and near ultraviolet. These crystals are essentially ionic in nature. The colour centers and also impurity centres produce optical absorption bands in the otherwise transparent crystals such as alkali halides, alkaline earth halides etc [6,7]. Colour center research on luminescent materials has led to many practical applications such as radiation dosimetry, high-density memory devices, tunable lasers etc.

The optical absorption due to F-centres in alkali halides generally fall in the visible region of the electromagnetic spectrum.. it is due to the 1s – 2p transition of the F-centre electron. The F-centre absorption is bell shaped and Gaussian. It is broad due to the strong interaction between the electron and the surrounding lattice.

In the present study UV-Vis absorption spectra were obtained and band gap energy, optical conductivity and Cole-Cole plot were drawn.

II. EXPERIMENTAL DETAILS

Mixed crystals of $Na_xK_{1-x}Br$ were grown from the aqueous solutions by the slow evaporation method for various values of x ranging from 0.1 to 0.9 along with two end member crystals NaBr and KBr for comparison purposes.

Refractive indices of all the crystals were determined using Abbey refractometer a Cary 5E UV-Vis-NIR spectrometer was used to measure the absorption spectra of the samples in the wavelength range of 200 to 800nm. The UV-Visible spectra of the material provide an important information about the details related with optical band gaps[8].

The optical energy gap (E_g) can be calculated from the well-known quadratic equation [9] which is often called Taue law

$$\alpha h\nu = A(h\nu - E_g)^n$$

where $h\nu$ = incident photon energy,
α = absorption coefficient,
E_g = band gap of the material,
A = constant that depends on the electronic transition probability and
n = an exponent that characterizes the type of electronic transition responsible for the optical absorption process.

For direct allowed transition n = ½, indirect allowed transition n = 2. To determine the possible transitions, $(\alpha h\nu)^n$ versus hν were plotted and corresponding band gap were obtained from extrapolating the straight portion of the graph on hν axis at α = 0. The absorption edge studies are important, especially in connection with the theory of electronic structure. In the present study it is found that n =1/2.

From the UV-Visible spectra, it is clear that the absorbance decreases with increase in wavelength. This decrease in the absorption indicates the presence of optical band gap in the material[10,11]

The optical conductivity σ is obtained using the relation [10]

$$\sigma = \frac{\alpha n c}{4\pi}$$

where c is the velocity of light in space, n is the refractive index and α is the absorption coefficient.

The dielectric constant can be obtained theoretically, since it was related to the absorption coefficient. The real part (ε_r) and the imaginary part (ε_i) of the dielectric constant was obtained using the relation[10]

$$\varepsilon_r = n^2 - k^2$$

and

$$\varepsilon_i = 2nk$$

Where n is the refractive index of the crystals and k is the extinction coefficient given by [10]

$$k = \frac{\alpha\lambda}{4\pi}$$

where λ is the wavelength of the incident light. The imaginary part of dielectric constant represents loss factor or energy absorbed.

So, the complex dielectric constant is given by

$$\varepsilon^* = \varepsilon_r - i\varepsilon_i$$

The graph between the ε_r(real part) and ε_i (imaginary part) is known as Cole-Cole plot[11].

III. RESULTS AND DISCUSSIONS

The absorption spectrum of the sample $Na_{0.5}K_{0.5}Br$ is shown in figure 1 for illustration. This spectrum shows a sharp increase in absorption at wavelength near 280nm, the absorption edge of the threshold wavelength for onset of absorption. The energy correspond to this determines the band gap of the material [10]. Refractive index, the threshold wavelength and band gap energy are provided in table 1.

The variation of $(\alpha h\nu)^{1/2}$ as a function of photon energy (hν) of equimolar crystal is shown in figure 2 for illustration.

It is found that the band gap energy decreases with increase in concentration of Na ions.

Figure 3 shows the variation of optical conductivity with incident photon energy for $Na_{0.5}K_{0.5}Br$ crystal. Optical conduction is constant up to 3.6 eV of photon energy. After that it increases rapidly with increase in photon energy. The increased optical conductivity at high photon energy is due to high absorption in that region.

The variation of real part and imaginary part of the dielectric constant for the sample $Na_{0.5}K_{0.5}Br$ is shown in figure 4 for illustration. This fit into a semi circle well.

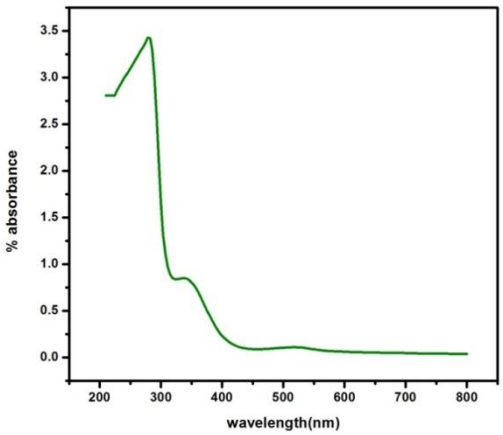

Figure 1. : UV absorption spectra of $Na_{0.5}K_{0.5}Br$ single crystal

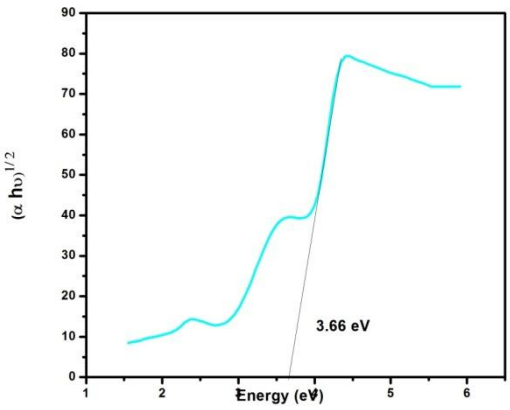

Figure 2: Plot of determination of optical bandgap of $Na_{0.5}K_{0.5}Br$ single crystal.

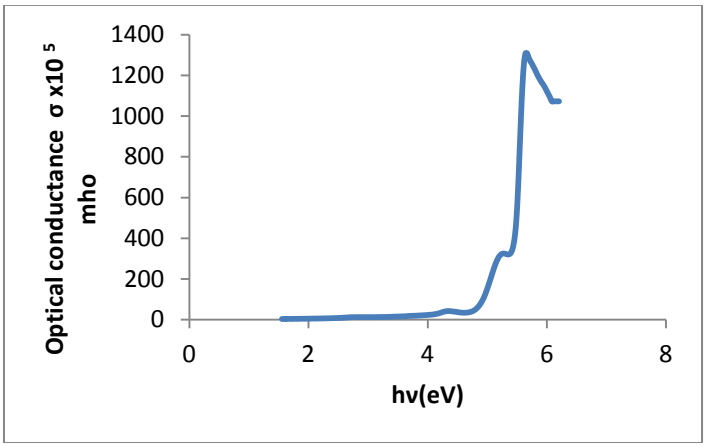

Figure 3. : Optical conductance of $Na_{0.5}K_{0.5}Br$ single crystal

Table1: Refractive index, the threshold wavelength and band gap energy for all the grown crystals.

System	Refractive index	Threshold wavelength (nm)	Band gap energy (eV)
KBr	1.554	210	4.49
NaBr	1.643	228	3.60
$Na_{0.1}K_{0.9}Br$	1.568	213	4.51
$Na_{0.2}K_{0.8}Br$	1.578	210	4.02
$Na_{0.3}K_{0.7}Br$	1.582	210	4.82
$Na_{0.4}K_{0.6}Br$	1.591	228	3.77
$Na_{0.5}K_{0.5}Br$	1.599	220	3.66
$Na_{0.6}K_{0.4}Br$	1.607	220	3.79
$Na_{0.7}K_{0.3}Br$	1.623	217	3.86
$Na_{0.8}K_{0.2}Br$	1.631	219	3.67
$Na_{0.9}K_{0.1}Br$	1.69	215	3.95

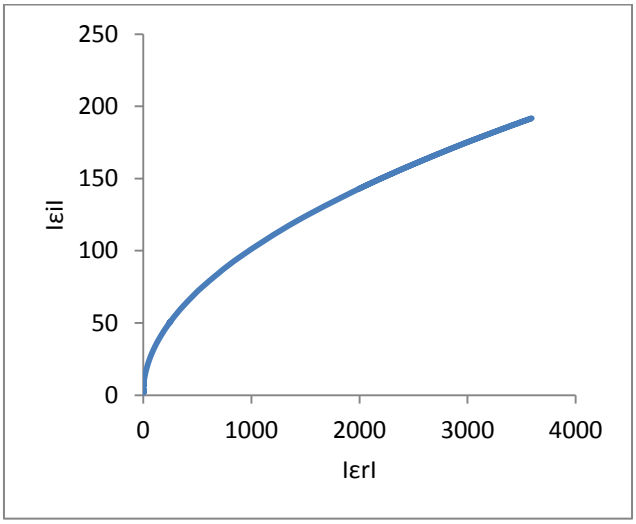

Figure 4. : Real and imaginary part of $Na_{0.5}K_{0.5}Br$ single crystal

IV. CONCLUSION

Binary mixed crystals of NaBr and KBr were grown from the aqueous solution by slow evaporation method. The optical band gap energy which was determined varies linearly with composition. The Taue plot shows that the allowed transition is direct. Optical conduction is constant up to 3.6eV of photon energy. After that it increases rapidly with increase in photon energy.

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