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Comparative Studies of Absorption and Mechanical Properties of Grown Alkali Halide Crystals

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Abstract: Absorption spectroscopy in the ultraviolet and visible region is widely used for quantitative determination of a large number of inorganic, organic and biological species while micro hardness test has been used as an alternative test for measuring material's tensile properties. The authors have studied the UV spectrum of NaF, NaCl and NaF: NaCl crystals, their relative plots and their band gap energies. The effect of temperature and load on the hardness of grown crystals has also been studied.
Keywords : Absorption spectra; UV spectroscopy; Energy Band Gap, Micro hardness, Mechanical Properties, Hardening Coefficient, Softening Coefficient.

Introduction and experimental

The band gap is an important parameter in semiconductor and nanomaterial industries. The band gap energy of insulators is large (> 4eV), but lower for semiconductors(< 3eV).The band gap properties of a semiconductor can be controlled by using different semiconductor alloys such as GaAlAs, InGaAs, and InAlAs.[1,2]Author has used UV- 2400PC series, Shimadzu spectrophotometer for absorption spectra of crystals at slit width 1.0 nm. Sample was scanned between UV-visible ranges (wavelengths from 200.0 nm to 800.0 nm) at sampling interval of 0.5 nm by Auto scanning mode. The author took 0.1 grams of NaF, NaCl and NaCl: NaF mixed crystals. Then dissolve them into 10 ml distilled water and made 1% solution of each. The standard sample was water. The UV spectrum of NaF and NaCl crystals are shown in Figure 1. Figure 2 shows the UV spectrum of NaF:NaCl mixed crystal. For classifying materials, hardness test are performed more frequently than any other mechanical tests. In the present work the micro hardness of the grown crystals is measured by Vaiseshika Vicker's micro hardness tester. Vickers Hardness is a measure of the hardness of a material, calculated from the size of an impression produced under load by a pyramid shaped diamond indenter [3]. The work hardening coefficient (n) of the material is related to the load (p) by the relation $P=ad^n$ ------ (1) , Where 'a' is an arbitrary constant. From Eq. -(1) log p=log a+n log d ---- (2).By comparing Eq-(2) with y= mx + c, y=log p, x=log d and m=n=slop of the graph [4-7].A relation between hardness of temperature was suggested by Ito & Shishiken in the form, H = A exp (-BT) --------(3) Where, H is the hardness equivalent to the mean compressive stress & the absolute temperature; A is known as the binding forces of the lattice. This is constant and correlation is sensitive to crystals structure. The constant 'A' is derived by extrapolating lnHv verses T/Tm like up to 0 K.

Constant B is called softening coefficient of hardness and is derived from the slope of the graph. After growing the crystal, the effect of temperature on the hardness of these crystals was studied. For this purpose, the heating coil is used. The line diagram of the coil is 0.5 cm with 6 cm in length. In order to determine the effect of temperature on the micro-hardness of NaF, NaCl and NaF:NaCl crystals, they were carried out from temperature 303 K at an interval of 5 K by keeping the load of 0.010 kg, loading time of 10 seconds[8-10]. The graph of Hardness vs. temperature are plotted as shown in Figure-3.Then the effect of different loads from 0.010 kg at the interval of 0.005 kg by keeping constant temperature and loading time of 10 seconds was studied [11-13].The graphs of Hardness Vs Load are plotted as shown in Figure-3. The work hardening coefficient and softening coefficient of the grown crystals were calculated from the graph of log p Vs log d and lnHv vs. T/Tm respectively.

Results and Discussion

From the spectra of each crystal, conclusion is drawn out that the maximum Absorption for NaF crystal is 0.036 at the wave length 222.50 nm, for NaCl crystal is 4.102 at the wave length 258.50 nm. and for NaCl:NaF mixed crystal is 0.203at the wave length 223.50 nm. Thus the maximum Absorptions for all these crystals are in between the wavelengths 200 nm to 400 nm which is ultra violet region and least amount of impurities are found in the above analysis. From the Table 1, conclusion can be carried out that the Band Gap Energy of NaF crystal is 5.02 eV and the Band Gap Energy of NaCl crystal is 2.55 eV. But the Band Gap Energy of NaF:NaCl mixed crystal is in-between NaF and NaCl crystals(3.29eV), while in the case of hardness, as the temperature increases, the hardness of the crystals decreases (Fig.3). For NaF Crystal, the Hardness becomes almost constant from 343 K., for NaCl Crystal, the Hardness becomes almost constant from 358 K. and for NaF:NaCl mixed crystal , Hardness becomes almost constant from 333 K. The softening coefficient of NaF NaCl and NaF:NaCl mixed crystals are found to be 32.47, 17.91 and 7.67. Thus the softening parameter B of mixed crystal is very low relative to that of NaF and NaCl crystals. The extrapolated intrinsic Hardness 'A' for NaF, NaCl and NaF:NaCl crystals are found to be 11.91,8.076 and 5.538 respectively. It is evident from the Fig.3, the HV value increases with load up to 0.035 grms for NaF crystal, 0.055 grms for NaCl crystal and 0.045 grms for NaF:NaCl mixed crystal and then the hardness tends to become constant and independent of load. It shows saturation beyond these loads and the value obtained from the saturation region, therefore, represents the true hardness of the materials. The hardening coefficients of NaF, NaCl and NaF: NaCl are 2.445, 3.828 and for 6.627 respectively.Thus the Work Hardening coefficient is very high for NaF:NaCl mixed crystal as compare to that of NaF and NaCl. Thus temperature and load are effective parameters for hardness of the crystal.

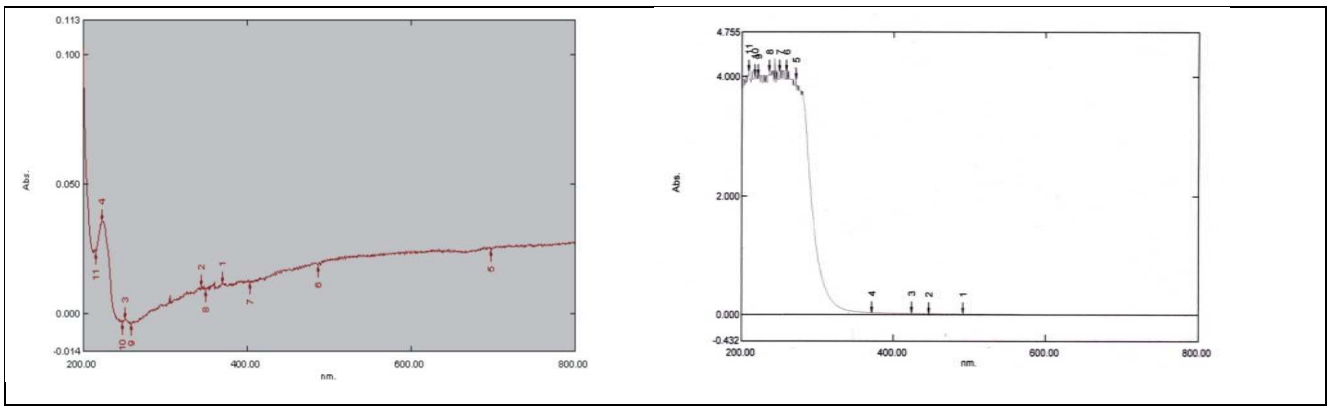

Figure 1: The UV spectrum of NaF, NaCl and NaF: NaCl crystals

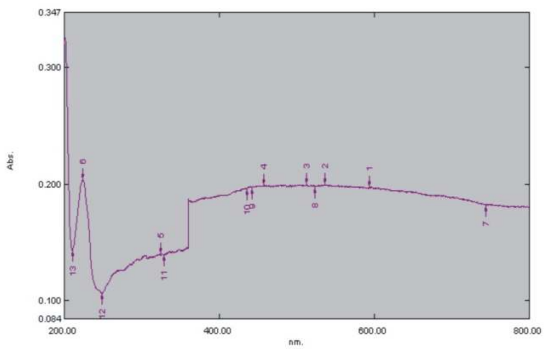

Figure 2: The UV spectrum of NaF: NaCl crystals

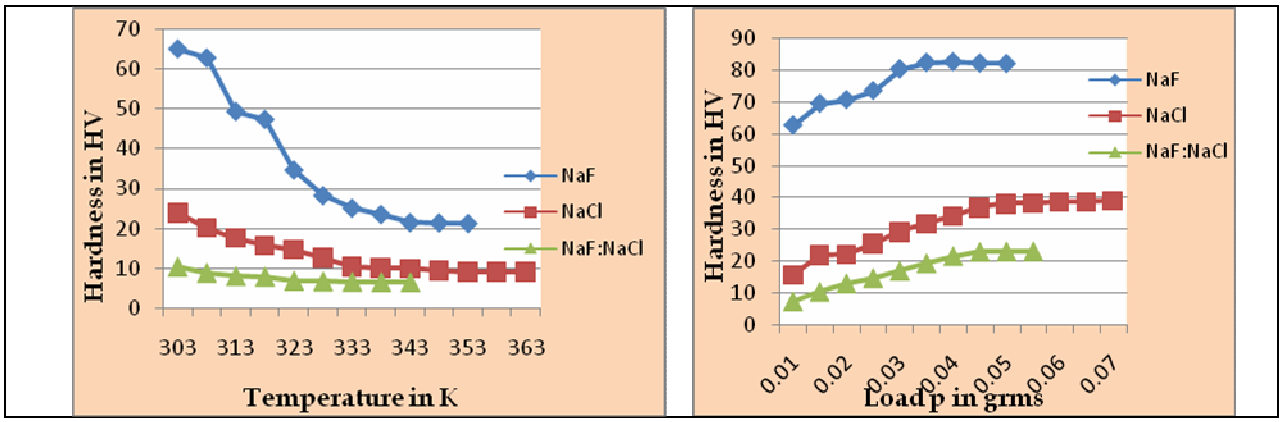

Figure 3: The graph of hardness vs. temperature and Hardness Vs Load

Table 1: Band Gap Energy of The grown Crystals

Crystal	λ	E in J	E in eV
NaF	2.48E-07	8.04E-19	5.02
NaCl	4.87E-07	4.08E-19	2.55
NaF:NaCl	3.78E-07	5.27E-19	3.29

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