Contribution ID: **363** Type: **Poster Presentation**

Characterization of defects in BaF2 using postron annihilation and XRD techniques

Wednesday, 5 July 2017 17:10 (1h 50m)

Different experimental techniques have clearly demonstrated that the predominant intrinsic point defects in ionic barium fluoride are anion Frenkel pairs. We utilized positron annihilation technique in obtaining Doppler broadening spectra in the temperature range 300 – 900 K. Theoretical approach uses the density functional theory and the generalized gradient approximation which calculate the Doppler broadening spectra. The Ba-atom contribution towards electron-positron annihilation momentum density increases steadily with temperature. At 693 K, the positron annihilation fraction due to Ba-atom when anion Frenkel is created, is found to be 84.44% compare to 15.56% for F-atom. We also noted that for F di-vacancy at 693 K, the annihilation fraction due to 5p and 6s valence and core electrons in Ba increases by 2.13% to 86.57%. The rate of disordering of fluorine sub-structure is found to increase non-linearly from a temperature of 580 K without observing any appreciable conductivity. X-ray diffraction method provided a lattice constant of 0.625 nm at 693 K through which an appreciable conductivity of 4.64 × 10-7 Ohm-1 cm-1 is first observed. This is demonstrated through the correlation between the lattice constants and the conductivity values at elevated temperatures.

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Session Classification: Poster Session 2

Track Classification: Track A - Division for Physics of Condensed Matter and Materials