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Study of lattice defects in BaF2 using positron annihilation and X-ray diffraction methods at elevated temperatures

Thursday, 11 July 2019 15:00 (2 hours)

We utilized positron annihilation technique in obtaining Doppler broadening spectra in the temperature range 300 – 900 K. Theoretical approach utilizes the Local Density and the Generalized Gradient Approximations that calculate the Doppler broadening spectra in the temperature range. We found that the positrons annihilating with barium valence electrons, especially the 5p and the 6s electrons, contribute immensely in the electron-positron annihilation momentum density. 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 intensity of disordering of fluorine sub-structure is found to increase non-linearly at a temperature from 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 small activity in the conductivity is first observed. This is demonstrated through the correlation between the lattice constants and the conductivity values at elevated temperatures.

Apply to be
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No

Level for award
 (Hons, MSc,
   PhD, N/A)?

N/A

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