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Vibrations of Impurity Iron Ions in Fluorides

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Annotation: In this work, temperature measurements of the gamma-resonance spectra of iron-57 isotopes were carried out. It is determined that the local Debye temperature for the replacement of iron ions in CaF_2 is two times higher than that of SrF_2.

Key words: Messbauer effect, resonant iron ions, Debye temperature, location of interstitial ions

Crystals with a MeF_2 fluorite like lattice (Me = Ca, Sr, Ba) exhibit super ionic conductivity at high temperatures [1]. They find wide practical application both in the super ionic and in the ordinary state. Crystals such as BaF_2 and CaF_2 are suitable materials for excimer laser optical components due to their ultraviolet transparency [2]. Bulk MeF_2 (Me = Ca,Sr,Ba) crystals doped with rare-earth metal ions have also been intensively studied for many years in a number of leading research centers in the world. Recently, the attention of researchers has been attracted by nano sized clusters of rare earth ions formed in these matrices [3]. Iron ions as impurities in the crystal activated by them can be of interest because their electronic structure is very sensitive to the crystal fields acting on them in the matrix crystal. Isolated divalent iron ions, ions can even be found in an exotic cubic environment not found in nature and artificial chemical compounds [4]. The use of multilayer crystalline systems in electronics and acousto electronics, often based on the resonant properties of such systems, requires an analysis of the features of the spectrum of vibrations of impurities in crystals. In this regard, the study of the vibrational properties of an isolated impurity depending on the location advances our knowledge in this area. In this work, temperature measurements of the gamma-resonance spectra of iron-57 isotopes in a system of doped MeF_2-Fe crystals were carried out in a wide temperature range (90-550K). The vibrational properties of ions have been analyzed depending on their location in the crystal lattice. This study had two goals:

a) Determination of the local Debye temperatures of impurity ions for various placement positions.

b) Determination of the dependence of the probability of recoilless absorption on the mass of the impurity and the mass of the matrix atoms. The oscillations of a resonant atom depend on the phonon spectrum of the lattice through the probability of recoilless absorption. In the Debye approximation, the probability is determined by the local Debye temperature for a given crystal position with a given atom.

$$W(T) = \frac{3E_R}{K\theta}\left[\frac{1}{4} + \left(\frac{T}{\theta}\right)\int_0^{\theta/T}\frac{xdx}{e^x - 1}\right]$$

In connection with the foregoing, changes in the normalized areas of the spectra of various impurity ions as a function of temperature are analyzed. The local Debye temperature for different crystallographic positions was found by approximating the temperature curve of the change in the ratio of the normalized areas under the partial spectrum. The obtained data on the local Debye

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temperatures are compared with the temperature change in the isomer shift and broadening of the lines of the partial spectra of substituting and interstitial iron ions [4]. As a result of the research, it was determined that the local Debye temperature for the replacement of iron ions in CaF_2 is two times higher than that of SrF_2. While for these matrices the Debye temperatures differ by 20% [5]. It may be worth considering the difference in metal-ligand distances. Moreover, this fact confirms the temperature change of the isomeric shift. For interstitial divalent iron ions in the SrF_2 matrix, an increased value of the local Debye temperature was found compared to the same ions in the substitution position, which is easily explained if we take into account that the atomic density is higher in the interstitial position in the first two coordination spheres [5]

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