Influence of Impurities on Liminescence Spectrum of ZnSe:Fe at Low Temperatures

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Abstract. A broad luminescence spectrum is presented, covering an energy range of 350-800 nm at temperatures of 18 K, 50 K, 90 K, 140 K, and 230 K. The sample ZnSe;Fe was excited by light with a wavelength of 325 nm (He–Cd laser). The resulting broad luminescence spectra at 18 K and 140 K were decomposed into Gaussian components, and the results were then thoroughly analyzed.

Keywords: Polycrystalline CVD ZnSe, Chemical Vapor Deposition, Iron impurities (ZnSe:Fe) crystals, High Isostatic Pressure (HIP).

1. Introduction

Recently, there has been increased interest in studying the influence of transition metals, including Fe^{2+} ions, on the electronic structure of zinc chalcogenides [1- 14]. Interest in this impurity was mainly due to its ability to reduce the efficiency of luminescence in the visible spectrum and expand the possibilities of using these materials as working media for IR lasers with a wide tuning range, as well as expand the possibilities of operation at room temperature (at T = 300 K) due to the formation of deep energy levels [4,5,6,8]. Transition elements, iron in particular, are centers that quench luminescence in the visible spectrum. Therefore, the study of the influence of iron ions on the optical properties of ZnSe in the visible spectrum is limited. At the same time, the calculation of the energy states of impurity iron ions in ZnSe indicates the possibility of radiative transitions with an energy close to the band gap of semiconductors [15]. Therefore, the study of the optical properties of ZnSe;Fe crystals in the visible spectrum is currently very relevant. in particular the study of luminescence associated with impurity defects in ZnSe:Fe at low temperatures is very important. In the present work, we analyze the PL spectra of ZnSe:Fe in a wide temperature range 18 - 230K.

2. Experimental Part

ZnSe:Fe sample was obtained using chemical vapor deposition (CVD) doped with iron. Fe^{+} film was deposited on both sides of the ZnSe samples obtained by CVD using electron beam

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evaporation, followed by diffusion doping using the HIP (hot isostatic pressure) method [8,11,12]. The obtained broad spectra at temperatures of 18K, 50K, 90K, 140K and 230K are shown in Figure 1. The spectra are excited using a He–Cd laser with the wavelength λ_{ex}=325 nm (so that the energy of exciting photon is larger than the bandgap, $h\nu_{ex} > E_g$).

Decomposition of broad luminescence spectra into Gaussian components (Fig.2,3) provides a complete analysis of the structure for each component of the luminescence centers. It is assumed that the diferences in the integrated spectra arise only due to a change in the relative contribution of the intensities of the individual components of the luminescence centers.

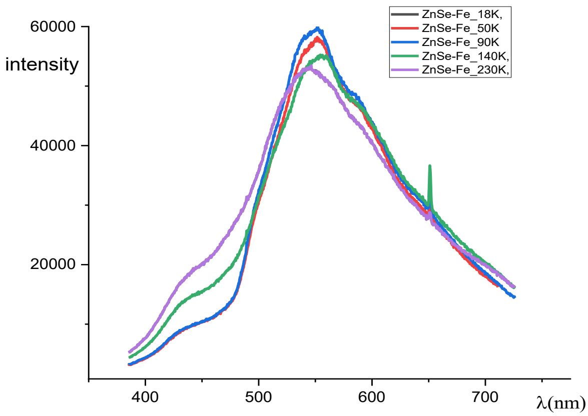

Fig. 1. Luminescence spectra of ZnSe;Fe at temperatures of 18K, 50K, 90K, 140K and 230K (*λex* = 325 nm)

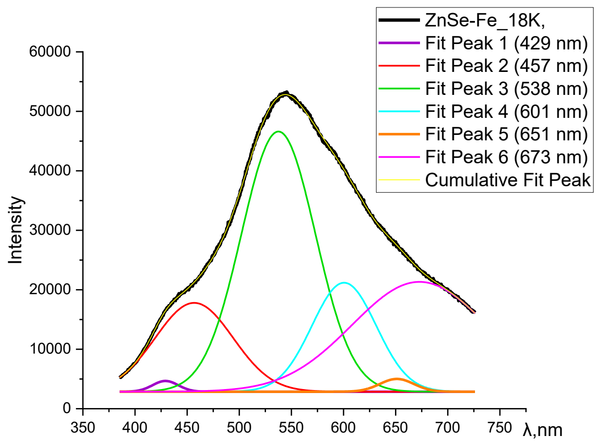

Fig. 2. Decomposition of luminescence spectra of ZnSe;Fe into Gaussian components at temperatures of 18K

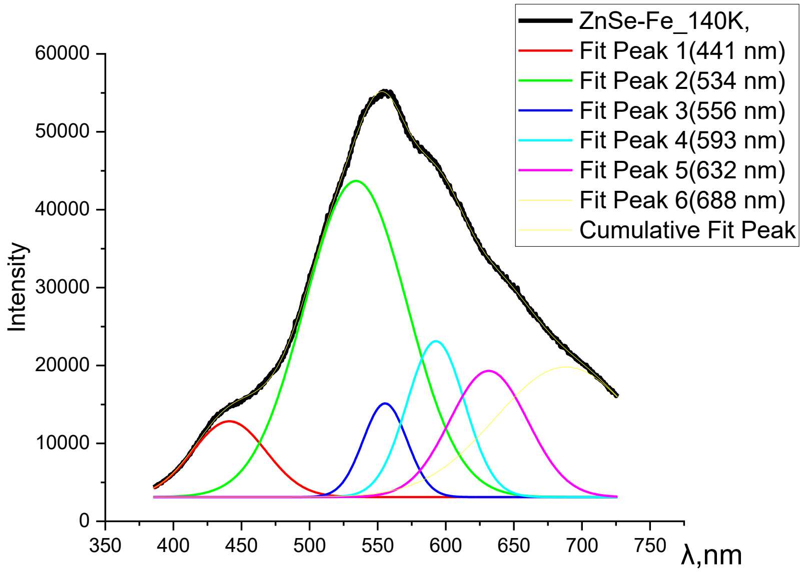

Fig. 3. Decomposition of luminescence spectra of ZnSe;Fe into Gaussian components at temperatures of 140 K.

3. Discussion of Results

Separating the luminescence spectrum (Fig. 1) at 18 K into Gaussian components (Fig. 2) reveals that this spectrum consists of maxima at 429, 457, 538, 601, 651, and 673 nm. The band at 429 nm is associated with emission from excitons localized at neutral zinc vacancies, while the band at 457 nm is associated with interband emission. The green band at 538 nm and the remaining red bands are associated with oxygen and copper impurities. When the temperature increases from 18 K to 140 K, the maxima in the luminescence spectra shift to the long-wavelength side. Dividing the luminescence spectrum (Fig. 1) at 140 K into Gaussian components (Fig. 3) shows that this spectrum consists of six maxima and the band of maxima is distributed as follows: 441, 534, 556, 593, 632 and 688 nm. The shift of the exciton maximum is 12 nm, which is consistent with the temperature-dependent change in the band gap with increasing temperature [9-11,16]. With increasing temperature, interband radiation disappeared (at 457 nm), and this also corresponds to literary data [9,10]. This indicates that band-to-band excitation of long-wave luminescence of ZnSe:Fe crystals is ineffective [10]. The main band at 18 K is green, with a maximum at a wavelength of 538 nm, at a temperature of 140 K it is observed at 541 nm, and it is obvious that mixing is insignificant.It is evident that with increasing temperature the proportion of low-energy bands increases, which is typical for intracenter luminescence [11,16]. Thus, it can be stated that the effective excitation of intracenter luminescence of ZnSe:Fe crystals is carried out by light from the region of intrinsic absorption of Fe+2 ions and in the low temperature range of 18-140K.

4. Conclusion

This study explores how iron impurities affect the photoluminescence properties of ZnSe crystals over a temperature range of 18–230 K using 325 nm excitation. The observed broad emission spectra (350–800 nm) were analyzed by separating them into individual Gaussian components, which revealed several luminescence centers linked to excitonic, interband, and impurity-related transitions. At low temperature (18 K), clear emission peaks were detected at 429, 457, 538, 601, 651, and 673 nm. As the temperature increased, these peaks shifted toward longer wavelengths, while interband emission gradually disappeared. The results show that luminescence is mainly governed by impurity-related intracenter transitions, especially those involving Fe^{2+} ions, which become more pronounced at higher temperatures. Overall, the findings demonstrate the important role of iron-induced energy levels in shaping the optical behavior of ZnSe and underline its potential for infrared optoelectronic applications.

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