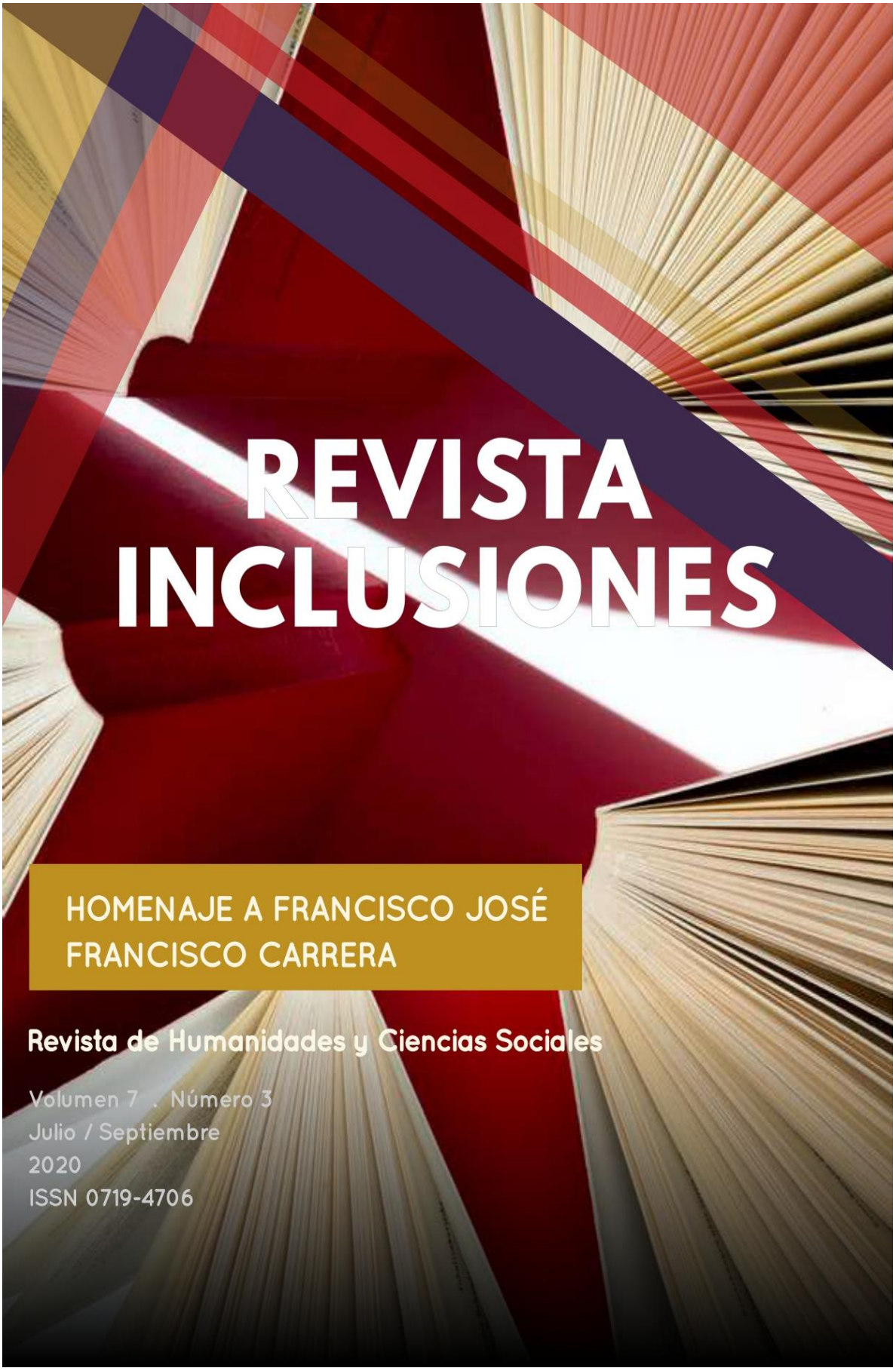
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THEORETICAL AND EXPERIMENTAL STUDIES OF THE SPECTRAL CHARACTERISTICS OF DOPED SEMICONDUCTORS USING ZINC OXIDE AND SULFIDE

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Abstract

In this work, we studied the spectral characteristics of the energy structure of Fe^{2+} ions in ZnO and ZnS semiconductor materials. The spectral characteristics of semiconductors doped with iron ions were obtained by direct matrix analysis. The wavelengths of the absorption bands obtained experimentally and according to the calculations showed a good correlation. The possibility of obtaining laser radiation on these materials in the range of 1.5 – 3 microns was evaluated.

Keywords

Semiconductors – Lasers – Iron ions – Energy structure – Transition intensities

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Introduction

Constantly increasing volumes of information transmitted by fiber-optic communication lines necessitate the expansion of the frequency range of transmitting radiation[1]. As the studies of a number of authors show, the search for methods of obtaining materials for radiation sources in the spectral range of 1.5–3 μm [2], especially those, which having frequencies different from those, which already used in existing devices, has a great practical importance [3].

As radiation sources, the most optimal are semiconductor lasers, which are characterized by a large range of generated power in continuous and pulsed modes and high speed with pulse modulation [4]. Also, their radiation frequency can be tuned within the luminescence area [5]. Compared to other types of lasers, they have the highest efficiency, smaller weight and dimensions [6]. $A^{II}B^{VI}$ semiconductors doped with Co^{2+}, Fe^{2+}, Ni^{2} ions are the subject of great interest for the construction of semiconductor lasers. Ions of this group have wide lines of absorption and emission spectra, which is interesting for reconfigurable mid-infrared lasers [7]. The work carried out in this field is mostly experimental, and is devoted to a single ion in a single semiconductor or a single ion in a small array of semiconductors [8]. Some works are devoted to individual types of semiconductors obtained by the diffuse method, as well as to repetitively pulsed lasers [9].

The general theory of the ligand structure of the environment of iron group ions was developed[10]. However, no methods have yet been developed for calculating the amplitude-

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spectral characteristics of the luminescence of iron group ions in semiconductors [11], taking into account all possible interactions of the fields in the ion and the interaction of the ion with the fields of ligand surroundings of various symmetries, which leads to significant difficulties in the development of semiconductor lasers [12].

The aim of this work is to calculate the parameters of the array of luminescence regions in Fe^{2+} ions introduced into $A^{II}B^{VI}$ semiconductors in the wavelength range (1.5–3) μm and to compare the calculation results with experimental ones [13].

Calculation of the position of absorption bands of an iron ion in semiconductors

The interaction matrix is based on the Hamiltonian, which describes the energy structure of the ion [14]. The Hamiltonian includes the following interactions: electrostatic interaction of electrons with each other Vqq, spin-orbit Hso and Hsf interaction [15], taking into account the effect inside the crystal field [16]. The Hamiltonian of these interactions for ions of the transition group of iron with electronic configurations $3d^7$, $3d^8$, $3d^6$ has the following structure: H = Vqq + Hsf + Hso [17].

The electrostatic interaction between electrons is responsible for the distribution of energy levels over multiplets with certain quantum numbers of the orbital *L* [18] and spin moment of the momentum *S* [19].

As a rule, in case of $A^{II}B^{VI}$ type semiconductors, symmetry of the active center of the crystal field is described as one who having a tetrahedral (T_d) and a trigonal part

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(C_{3v})[20], which defines a set of parameters of the crystal field with values of k, q = 2, 0; 4, 0; 4, 3; 4, -3 [21]. But it is more convenient to use the well-known parameters of the crystal field corresponding to the pure tetrahedral (parameter *Dq*) [22] and trigonal (parameters D_E) components of the crystal field potential [23].

The interaction operators in the Hamiltonian are expressed in terms of the following parameters [24]: ξ_d is the spin-orbit coupling constant, A_{20}, A_{40}, A_{44} are the interaction parameters with the crystal field potential of tetrahedral (T_d) symmetry (*Dq)* [25], and D_{2E}, D_{4E} are the parameters of low symmetry of the crystal field potential [26].

From the results of the study (Figure 1), Fe^{2+} ions in ZnO show the largest number of transitions (five) with a wavelength in the target region of 1.3 - 3 μm [27], in CdO and ZnS (with three transitions) [28]. It was found that Fe^{2+} ions in ZnSe have one transition located within the studied range and two transitions in close proximity to the boundary of the target region [29], while ions in CdSe, CdTe, and ZnTe have no transitions with a wavelength in the target region [30].

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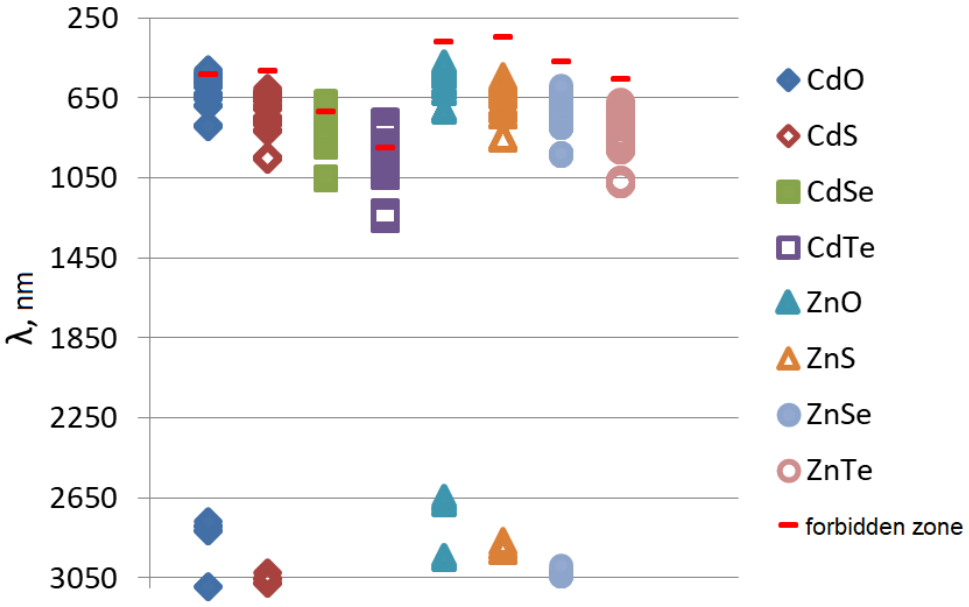

Figure 1
Wavelengths of transitions of Fe^{2+} in $A^{II}B^{VI}$ semiconductor array [31]

Iron ions in $A^{II}B^{VI}$ semiconductors also have fewer transitions within the transparency window of the corresponding semiconductors [32]. So, Fe^{2+} ions in Cds, as well as in all zinc compounds (ZnO, ZnS, ZnSe, ZnTe) [33] do not have transitions outside the band gap [34]. Fe^{2+} ions have three transitions in CdO, nine transitions in CdSe and ten transitions in CdTe [35].

Iron compounds have a total of fourteen transitions in compounds with the studied semiconductors [36], twelve of them have a relatively high oscillator strength to be used as laser materials [37].

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Table 1 compares the positions of the experimentally measured absorption bands of the Fe^{2+} ion in the ZnS semiconductor with the bands obtained theoretically using the above mentioned method [38].

	Fe^{2+} ion in ZnS			
Transition	Experiment	Calculation data		
		Bands with high oscillator strength		Wide band with low oscillator strength
$^5D_3$	2800	2891	2915	2868
$^5D_2$	3700	3536	3239	3218

Table 1

Position of the absorption bands obtained by theoretical and experimental method, nm [39]

The oscillation of the boundaries of the absorption bands obtained by the theoretical and experimental methods within 50-100 nm is explained by the difference in data [40]: if the position of the peak of the spectrum was measured in the experiment, the theoretical method gives the position of the transitions that form the spectrum and requires further approximation [41]. The magnitude of the fluctuations is 3-5%, which proves the adequacy of used mathematical model [42].

Conclusions

Using matrix analysis, it was possible to detect the presence of a discrete transition, which is difficult to determine during experimental observation, and to obtain information about its location in the spectrum. This method can be applied in a similar way to a wide array of ions and semiconductors, as an auxiliary reference tool in the design of semiconductor lasers.

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