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COMPUTER SIMULATION OF ENERGY TRANSFER: APPLICATION TO THE PHOTOLUMINESCENCE IN CdMnTe

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The transfer is studied on an fcc-lattice filled at random with optically active ions. The computed results for time-resolved emission are compared with experimental data.

We report on a computer simulation of the radiationless energy transfer[1] between Mn^{2+}-ions in the semimagnetic semiconductor $Cd_{1-x}Mn_xTe$. The model was applied to explain the photoluminescence properties in this material and in other II-VI-semiconductors with high manganese concentration, which were investigated by cw- and pulsed excitation.[2)3)] An fcc-lattice with 4096 lattice points and periodic boundary conditions is randomly occupied with "active" ions corresponding to a molar concentration of manganese x. The active ions are given 2 electronic states with energies E_g and $E_e = E_g + E_o + N \cdot \Delta E$, where N is the number of "active" neighbors. The expression for E_e simulates the random crystal field seen by one active ion. The simulation

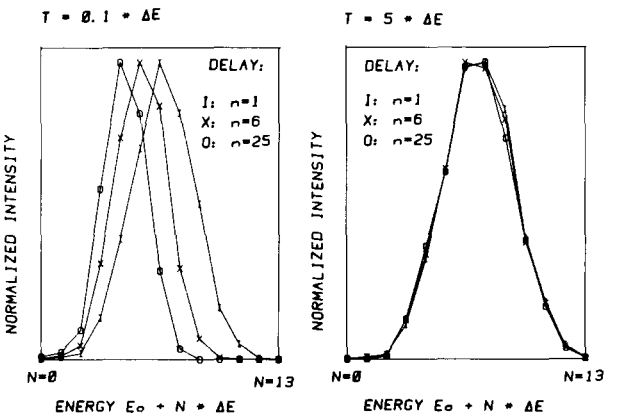

Fig. 1

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starts with the excitation of a random active lattice point x. After an internal time interval Δt the excitation either decays with a certain probability W by photon emission or is transfered to a random neighboring active lattice point x'. If it has to step up in energy, the transition probability is equal to $\exp \frac{(E_e(x)-E_e(x'))}{k_B T}$, if it steps down, the transition probability is one. This procedure is repeated until the excitation decays radiatively with energy E(x') after n time intervals Δt. After 500 000 excitations the time resolved spectrum is determined from E(x') and n, which is equivalent to the delay time in the time resolved luminescence experiment. The spectra depend on temperature and delay time.

Fig. 1 shows two spectra plotted as a function of spectral energy and delay time. At low temperatures $T \ll \Delta E$ the redshift and band narrowing increases with delay time as was observed in the experiment.[2] At high temperatures $T \gg \Delta E$, redshift and narrowing vanish.

In Fig. 2 the emission intensity is plotted as a function of time after excitation for low temperatures $T = 0.1\ \Delta E$. The low energy emission shows

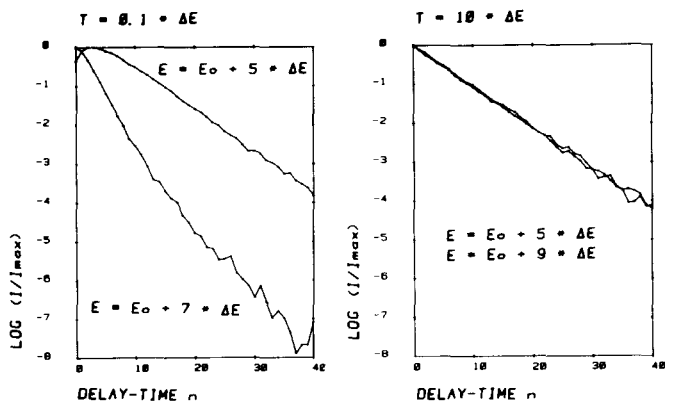

Fig. 2

an exponential decay for $n > 5\ \Delta t$, while the high energy emission does not. For $T = 10\ \Delta E$ the low and high energy emission can be fitted by a single exponential.

The results of the simulation agree qualitatively well with the experimental data obtained with $Cd_{0.5}Mn_{0.5}Te$. The simulated band narrowing after the time $25 \cdot \Delta t$ is about $2 \cdot \Delta E$. When we compare this with the experiments[3]

we obtain $\Delta E \approx 100\ cm^{-1}$. This is unfortunately too high to account for the observed temperature effects. The simulation also gives a cw-bandshift with temperature $\frac{dE}{dT}$ which is monotonous and always positiv. However the observed bandshift shows a pecularity: $\frac{dE}{dT}$ is negativ below 60 K and positive above.[2] In our opinion it is the description of the random crystal field which is too simple to account for the cation interaction in $Cd_{1-x}Mn_xTe$. It is well known from magnetic measurements that the exchange interaction between Mn^{2+}-ions leads to spinglass properties below 30 K and a temperature dependent spin arrangement.[4)5)] This would make ΔE much smaller and temperature dependent.

The merit of the present simulation is to show how far simple assumptions can be used and what kind of improvements we have to consider for a more realistic treatment.

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