STUDIES OF SELF-TRAPPED EXCITON LUMINESCENCE IN Csl

J.P. Pellaux, T. lida* and M.A. Aegerter
Institut de Physique, Université de Neuchâtel
CH 2000 NEUCHATEL, Switzerland

Self-trapped exciton (STE) luminescence is observed in all pure alkali halides exposed to X-ray or UV excitation and the occurence of these emissions when Vj£ centers and electrons recombine led to the identification of the (VK + e~) center as the STE. In Csl two emissions are observed peaking at 290 nm and 338 nm. At low temperature both bands have a complex behaviour but appear as concurrent, the sum of their intensities being constant.

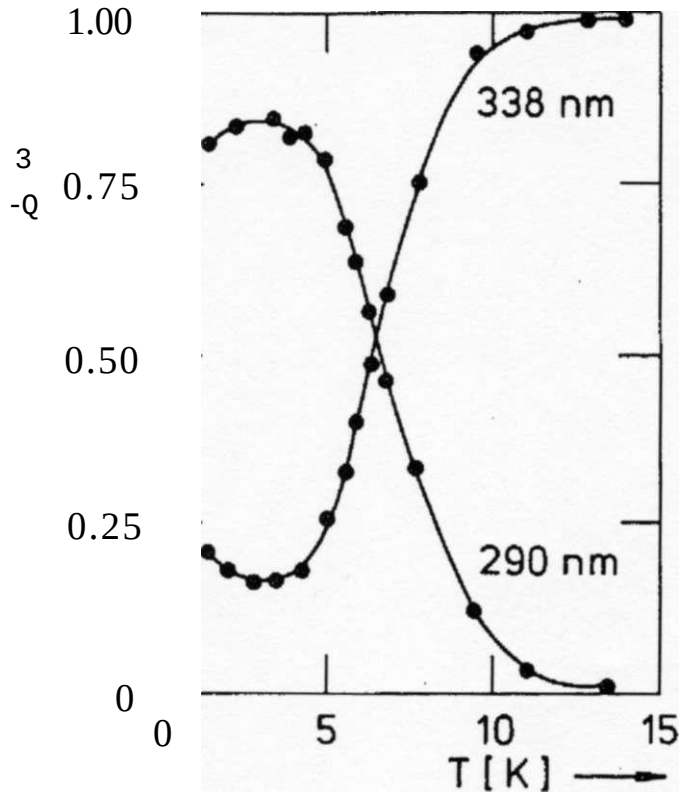

Fig- 1
Temperature variation of the normalized intensities of the 290 nm and 338 nm emission of STE in Csl.

A theoretical model for the relaxed STE in CsCl structure has been worked out by considering the electronic states of a cluster composed of an anionic diatomic molecule Xg" surrounded by 12 alkali ions in a D^^ symmetry. Excitation of this cluster leaves an electron in a r£ or Tg state with a hole in a or rjj state. Assuming that relaxation processes do not change the overall D^ symmetry and taking into account the spin-orbit interaction up to 2ⁿ‹i order perturbation the various excitonic states can be constructed. Two kinds of STE state manifold are obtained. Both of them are composed of a partially allowed triplet state below a singlet one. (Fig. 2)

On the basis of experimental results we have attributed the mani-fold to the 290 nm emission (**ir** + *a* polarized) and the 1^ manifold to the 338 nm emission (only **IT** polarized). A thermal and athermal process connecting both kinds of STE states can account for the temperature behaviour of both emissions. Other experiments have been done in order to test the model [1] : optical, ESR and theoretical investigations show that VK centers

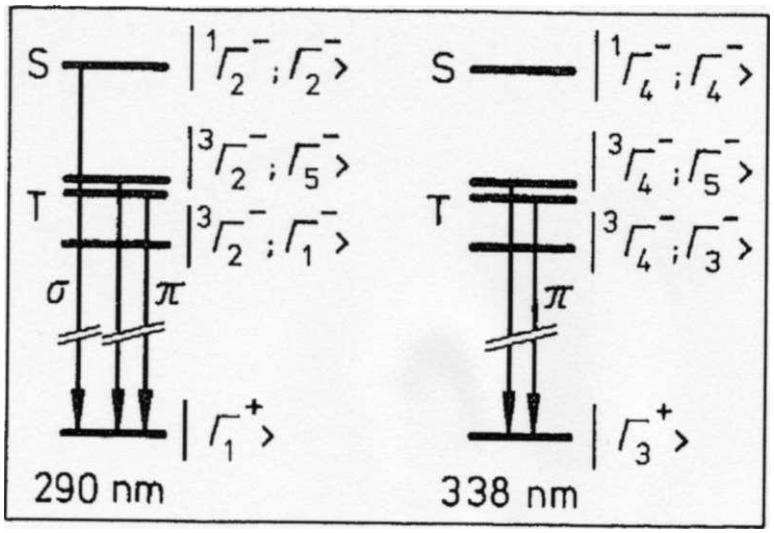

Fig. 2
The lowest levels and the allowed transitions of the two types of STE in CsI. The symmetry of the levels are labelled as |orbital function⟩|total function⟩.

can be almost completely aligned for T < 60 K in a [100] direction by optical excitation in their -*•²£g UV transition *(klO* nm). The (V_K-e~) recombination should then appear linearly polarized.

Experimental results confirm it only partially. The 338 nm emission polarization is independent of temperature as it should be but its value is only *26%* instead of 100$ as foreseen. The 290 nm emission polarization decreases as the temperature increases due to thermal population transfer to the singlet state but its maximum value at LHeT is only We therefore postulate that an athermal reorientation process of the bound e"~-hole pair occurs during their relaxation in higher excited states of the STE. In our case *k5%* of the exciton created with a fully aligned center system reorient along the two other <100> directions. This is in agreement with recent observations of STE emission in KC1 by Purdy et al. [2] and Williams [3] . Using reasonable values for the other parameters we shall show that it is possible to fit the experimental data including the temperature dependence of intensities, linear polarizations and decay times of both emissions.

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References

* Now at Osaka City University, Sumiyoshi-ku, Osaka, Japan.

[1] See also other abstract by L. Falco, J.P. von der Weid and M.A. Aegerter

[2] A.E. Purdy, R.B. Murray, K.S. Song and M.A. Stoneham, Phys. Rev. 15, 2170 (1977)

[3] R.T. Williams, Phys. Rev. Lett. 36, 529 (1976).