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UV-visible emission of (Cl^-)* color centers in NaCl single crystals grown by Czochralski method

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ABSTRACT

The (Cl^-)* color centers inside the single crystals of NaCl have been studied. The single crystals have been performed using the Czochralski method. The photoluminescence and the photoluminescence excitation spectra showed the emission bands of (Cl^-)* centers in NaCl situated in the UV-visible range.

KEYWORDS

NaCl single crystals;
(Cl^-)* color centers;
Photoluminescence.

INTRODUCTION

When Pohl[1] started research on the alkali halides in the nineteen-twenties, it was hoped that the knowledge obtained from these materials would add to the understanding of solids as a whole. It was found, however, that they show some extreme properties (strongly ionic character and large energy gap). Which make them stand apart from the solids of more commercial interest such as the semiconductors. These materials have nevertheless been made the subject of a great number of investigations because of their interesting properties and their ease of purification and crystallization. A large part of alkali halides have been devoted to the color centers.

During the past few years, color centers in alkali halides have received attention because of their usefulness as laser active centers[2,3]. It was recently reported the development of a new color center in NaCl single crystals excited in the UV range, based on what we tentatively identified as an (Cl^-)*[4]. This center represents an interstitial position of Cl^- ion in the crystal lattice of alkali halides like KCl and NaCland it is produced by the displacement of Cl^- ion from their normal sites.

In this paper, the author has elaborated the single crystals of NaCl and hasstudied their optical properties in order to show the emission bands of (Cl^-)* center in NaCl.

EXPERIMENTAL

The NaCl single crystals were prepared by using the Czochralski method in free atmosphere in Laboratoryof Crystallography (LC) at the Constantine University in Algeria. The powder of NaCl is provided by Panreac Quimica Company in Spain. The single crystals are cleaved perpendicular to the direction [100] in order to prepare samples with 1 mm thickness. Some samples have been annealed at 650°C for 24 h and then cooled slowly at room temperature.

Photoluminescence spectra (PL) were recorded at

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78 K by using a Jobin-Yvon spectrometer HR 460 provided of CCD (Charged Coupled Device). The source of excitation in the UV-visible range is a xenon lamp (450 W). However, the photoluminescence excitation spectra (PLE) were measured at 78 Kwith a Jobin-Yvon spectro-fluorometer Fluorolog-3, using a xenon lamp 450 W.

RESULTS AND DISCUSSION

Figure 1 shows the emission spectra of our samples excited with 270 nm at 78 K before and after annealing. A series of emission lines between 500-800 nm have been observed, which are assigned to the electronic transitions from the lowest vibrational levelof the excited state $^2\pi_u$ to vibrational levels of the ground state $^2\pi_g$ of O_2^- molecule ions[5,6]. The oxygen is introduced inside the single crystals of NaCl because they are elaborated in free atmosphere[7]. Before annealing (Figure 1.a), the spectrum presents two emission bands, situated at 350 nm and 460 nm. After annealing (Figure 1.b), the 350 nm band become very intense and shifted by 30 nm. It is now located at 380 nm. While, we note a large emission band situated between 500-800 nm and centered at 620 nm (see the inset Figure 1). This band is determined using the Gaussian fit. In order to prove the appearance of an emission band centered at 620 nm, we have measured the PLE at 620 nm before and after annealing (Figure 2). The spectra show that after annealing, the excitation band become very intense and located at 271 nm.

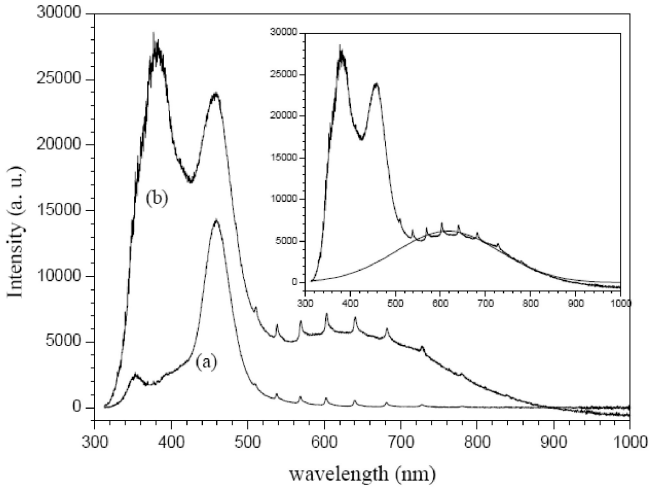

Figure 1 : Emission spectra of NaCl excited with 270 nm and measured at 78 K: (a): before annealing, (b): after annealing. The inset shows the emission band 620 nm.

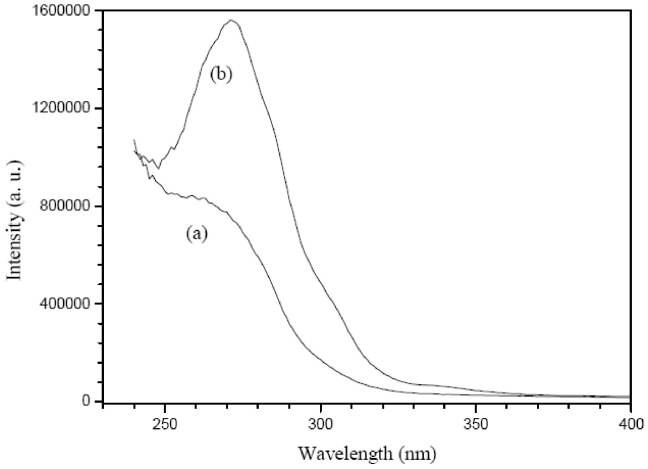

Figure 2 : Excitation spectra of NaCl measured at 620 nm and obtained at 78 K: (a): before annealing, (b): after annealing.

Figure 3 displays the PL spectra of samples excited with 360 nm at 78 K, before and after annealing. The spectra present a large emission band between 400-550 nm, formed by four peaks,each one situated at 415, 440, 460 and 500 nm. After annealing, we observe that the large emission band is become very intense. It is probably due to the increase of the point defects because of the thermal agitation of atoms inside the lattice of single crystals during the annealing. The PLE spectra measured at 380, 460 and 500 nm after annealing,are illustrated in Figure 4. We noticedan excitation band situated about 271 nm. However for 500 nm, we observe a weak excitation band as show by the arrow. The position of this band is determined by the second

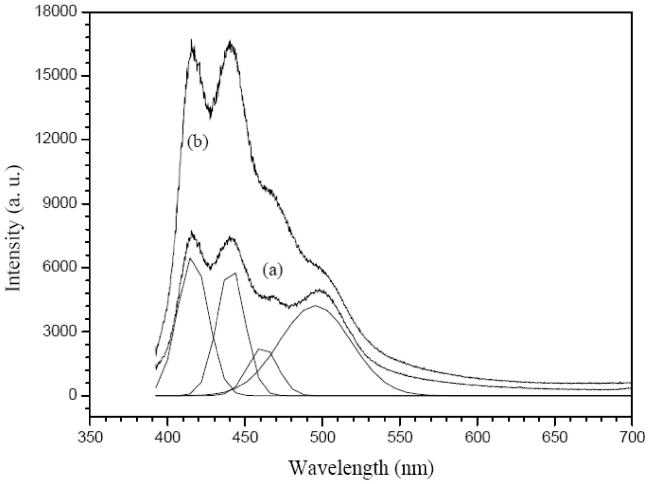

Figure 3 : Emission spectra of NaCl excited with 360 nm and measured at 78 K: (a): before annealing, (b): after annealing.

derivative method is equal to 284 nm (see the inset Figure 4) and it is assigned to (O^{2-} - F^{+}) centers[8]. This center is formed from the reaction between the F and the O_2^- centers as follow:

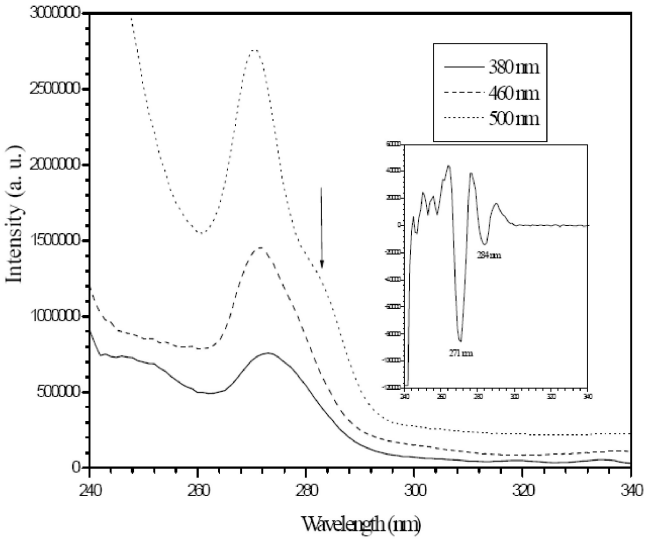

Figure 4 : Excitation spectra of NaCl measured at 380, 460 and 500 nm after annealing and obtained at 78 K. The inset shows the second derivative method.

$O_2^- + 3\,F \rightarrow 2(O^{2-} - F^{+})$

In term of adiabatic potential energy surface and Jahn Teller effect, J. G. Kang has assigned the 271 nm excitation band to the electronic transition from the ground state $^1A_1$ to the excited states $^3A_1$ of (Cl^-)* centers[4].

CONCLUSION

In this paper, the (Cl^-)*centers inNaCl single crystals have been investigated, which are elaborated by the Czochralski method. A comparison study between our results and those obtained by J. G. Kang, permits to deduct that the emission bands peaking at 350, 380, 415, 440, 460, 500and 620 nm in NaCl crystals are due to (Cl^-)* centers.

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