IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

A note on the origin of the yellow luminescence in GaN

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1998 J. Phys.: Condens. Matter 10 L461

(http://iopscience.iop.org/0953-8984/10/27/003)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.209
The article was downloaded on 14/05/2010 at 16:35

Please note that terms and conditions apply.

J. Phys.: Condens. Matter **10** (1998) L461–L463. Printed in the UK PII: S0953-8984(98)92406-7

LETTER TO THE EDITOR

A note on the origin of the yellow luminescence in GaN

B K Ridley†

School of Electrical Engineering, Phillips Hall, Cornell University, Ithaca, NY 14853-5401, USA

Received 11 March 1998

Abstract. The broadband yellow luminescence frequently observed in GaN is shown to be consistent with transitions to a single level strongly affected by Franck–Condon effects. A level 0.6 eV above the valence band with an associated Huang–Rhys factor of 6.5 determined by the electron–phonon polar interaction fully describes the breadth of the observer band.

The yellow luminescence commonly observed in GaN manifests itself in a broad band peaking at a photon energy of about 2.2 eV. *Prima facie*, this suggests the presence of a deep trap situated 1 eV from one or the other band edge or, to account for the large bandwidth, a range of traps spread around 1 eV. An alternative explanation is suggested here based on a simple model. The existence of a single type of centre is proposed situated in energy about 0.6 eV from the valence band edge and which interacts with the polar optical vibrations strongly enough to produce a Stoke's shift of about 1.2 eV. Such a Stoke's shift accounts for 0.6 eV to be dissipated by phonons in the radiative transition. This corresponds to a Huang–Rhys factor of 6.5 (with a phonon energy of 92 meV). The energy of the photon emitted in luminescence is then:

$$h\nu = E_{c,v} - E_T - S\hbar\omega \approx 2.2 \text{ eV}$$

and the full width at half maximum is about $S\hbar\omega$ i.e. 0.6 eV at temperatures where the phonon occupancy number $n(\omega)$ is small. This compares well with a measured FWHM of 0.59 ± 0.02 eV at room temperature ($n(\omega) = 0.03$) [1]. The model used consisted of assuming that the centre was neutral and that the wavefunction of the trapped carrier was described by the quantum-defect form. The Huang–Rhys factor was calculated using this wavefunction and the polar interaction with LO phonons.

The Huang–Rhys factor is given by [2]

$$S = \sum_q \frac{D^2(q)}{2(\hbar\omega)^2 N} G^2(q) \tag{1}$$

where the sum is over all phonon modes, $\hbar\omega$ is phonon energy, N is the number of primitive unit cells, $D(q)$ is the interaction strength and $G(q)$ is the overlap integral. For the polar interaction:

$$D^2(q) = \frac{e^2\hbar\omega}{V_o q^2}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s}\right)\begin{cases} n+1 \\ n \end{cases} \tag{2}$$

† Present address: Department of Physics, University of Essex, Colchester CO4 3SQ, UK.

0953-8984/98/270461+03$19.50 © 1998 IOP Publishing Ltd

where V_0 is the volume of the unit cell, q is the phonon wavevector, ε_∞, ε_s, are the high-frequency and static permittivities, and n is the phonon-occupation factor. The overlap integral is:

$$G(q) = \int \psi^2(\boldsymbol{r}) \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\,\mathrm{d}\boldsymbol{r} \tag{3}$$

and the wavefunction of the trapped carrier is described by the quantum-defect model [3]:

$$\begin{aligned} \psi(\boldsymbol{r}) &= u_\alpha(\boldsymbol{r}) F(\boldsymbol{r}) \\ F(\boldsymbol{r}) &= A\left(\frac{2r}{\nu a}\right)^{\mu-1} \exp\left(-\frac{r}{\nu a}\right) \\ \nu &= \left(E_H/E_T\right)^{1/2} \qquad \mu = Z\nu \qquad A = \left[4\pi(\nu a/2)^3 \Gamma(2\mu+1)\right]^{-1/2} \end{aligned} \tag{4}$$

where $u_\alpha(\boldsymbol{r})$ is the cell periodic wavefunction for the conduction band ($\alpha = c$) or valence band ($\alpha = v$) edge, a is the effective Bohr radius, E_H is the effective hydrogenic donor or acceptor energy and Z is the number of charges. This model has been used very successfully to describe photoionization of hydrogenic ($\gamma = 1$, $z = 1$) and neutral ($Z = 0$) centres [2]. Attention will be limited to these types of centre.

The overlap integral is given by:

$$\begin{aligned} G(q) &= \frac{\Gamma(2\mu)}{\Gamma(2\mu+1)} \frac{\sin(2\mu \tan^{-1}(q\nu a/2)}{(q\nu a/2)(1+(q\nu a/2)^2)^\mu} \\ &= \frac{1}{(1+(q\nu a/2)^2)^2} \qquad \mu = 1 \\ &= \frac{\tan^{-1}(q\nu a/2)}{(q\nu a/2)} \qquad \mu = 0. \end{aligned} \tag{5}$$

For temperatures up to room temperature it will be sufficient for GaN to assume $n = 0$ and calculate S at $T = 0$. The sum over phonon modes can be converted to integral form in the usual way, assuming a spherical Brillouin zone of radius $q_D = (6\pi)^{1/3}/a_0$ where a_0 is the unit cell dimension ($4^{-1/3}$ multiplied by the lattice constant). We obtain for hydrogenic centres:

$$\begin{aligned} S &= 0.16 \text{ electrons } \left(m^* = 0.2m_0\right) \\ &= 0.78 \text{ holes } \left(m^* = 1m_0\right). \end{aligned} \tag{6}$$

For neutral centres the Huang–Rhys factor depends on the radius of the wavefunction:

$$S = 20.57\left(E_T E_H\right)^{1/2}. \tag{7}$$

Thus

$$h\nu = E_g - E_T - S\hbar\omega. \tag{8}$$

Solving for E_T we obtain:

$$\begin{aligned} &\text{for electrons: } E_T = 0.88,\ S = 3.5 \\ &\text{for holes: } E_T = 0.60,\ S = 6.5. \end{aligned} \tag{9}$$

These figures suggest a FWHM of 0.32 eV for electrons and 0.60 eV for holes. The latter fits the observed value.

The calculation was also carried out for the deformation potential interaction. Significantly smaller values of S were obtained.

Given the crudity of the model these quantitative results must be regarded as rough estimates, but qualitatively at least, the origin of the yellow luminescence and its large

bandwidth appear to be explainable on the basis of a Franck–Condon effect associated with a centre whose energy level is within 1 eV of the valence band edge. This conclusion is consistent with the result derived from measurements of photocapacitance [4]. The nature of the centre remains unknown.

This work was supported by ONR MURI Grant #00014-96-11223.

References

[1] Eastman L F 1998 private communication

[2] See, for example, Ridley B K 1993 *Quantum Processes in Semiconductors* 3rd edn (Oxford: Oxford University Press) pp 202–8, 256–63

[3] Bebb H B and Chapman R A 1971 *Proc. 3rd Photoconductivity Conf.* ed E M Pell (Oxford: Pergamon) p 245

[4] Calleja E, Sanchez F J, Basak D, Sanchez-Garcia M A, Munoz E, Izpura I, Calle F, Tijero J M G, Sanchez-Rojas J L, Beaumont B, Lorenzini P and Gibart P 1997 *Phys. Rev.* B **55** 4689