University of Essex

Effect of non-parabolicity on the density of states for high-field calculations in dilute nitrides

Department of Electronic Systems Engineering

M. P. Vaughan and B.K. Ridley

Optoelectronic Materials and Devices Group, Dept. of ESE, University of Essex, Colchester, CO4 3SQ

Abstract

Using the 2-level band anticrossing (BAC) model [2] or its generalisation to *n*-bands [7-9], the essential features of the non-parabolicity of the band structure in dilute nitride materials can be captured using a **k.p** – like formulation. However, the derived densities of states in both 3D and 2D are then badly behaved near the nitrogen impurity levels with unrealistic consequences. Densities of states in the general *n*-band case are derived using a Green's function approach, which are well-behaved and conserve the number of states in the crystal.

The dispersion relations

The dispersion relations can be for an *n*-band model can be found from [7-9] (see figure 1 for details)

$$\begin{vmatrix} E-E_M & \beta_1 x_1^{1/2} & \beta_2 x_2^{1/2} & \cdots & \beta_{n-1} x_{n-1}^{1/2} \\ \beta_1 x_1^{1/2} & E-E_1 & 0 & \cdots & 0 \\ \beta_2 x_2^{1/2} & 0 & E-E_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ \beta_{n-1} x_{n-1}^{1/2} & 0 & 0 & 0 & E-E_{n-1} \end{vmatrix} = 0, \quad (1)$$

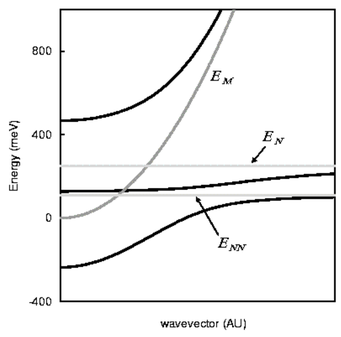

Figure 1 The dispersion relations in a dilute nitride material using a 3-band model. Here E_1 and E_2 from Eq. (1) are the isolated N and N-N pair environments (here denoted by E_N and E_{NN} respectively).

The values of these energy levels and the interaction elements are taken from ref [8]:

E_1 = 250 meV and E_2 = 110 meV (relative to E_M = 0), β_1 = 2450 meV and β_2 = 2650 meV. The concentrations are given by

$x_1 = x(1 - 12x)$ and $x_2 = 6x^2$.

Green's function approach

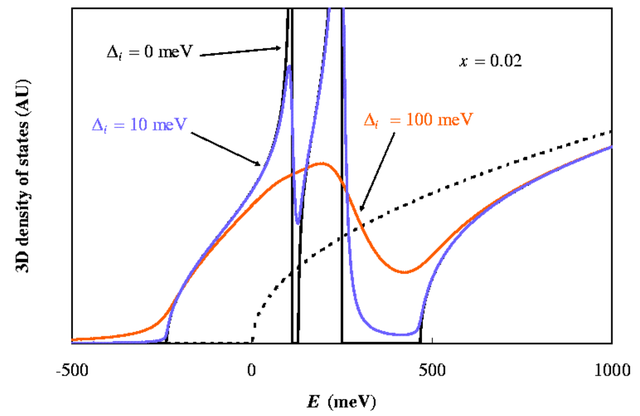

Figure 2 The 3D density of states for a 3 band model (see figure 1). The dotted line shows the matrix semiconductor density of states.

The non-parabolicity can be incorporated into a function of energy

$$\gamma(E) = \frac{\hbar^2 k^2}{2m^*}. \quad (2)$$

From Eq. (1), we find

$$\gamma(E) = \sum_i \frac{\beta_i^2 x_i}{E_i - E} + E. \quad (3)$$

Equation (1) can be reproduced from the poles of *

$$G(E, E_M) = \left\{ E - E_M(\mathbf{k}) - \sum_j \frac{\beta_j^2 x_j}{E - E_j + i\Delta_j} \right\}^{-1}. \quad (4)$$

Defining

$$\Omega(E) = -\sum_j \Omega_j(E), \quad \Omega_j(E) = \frac{\beta_j^2 x_j \Delta_j}{(E - E_j)^2 + \Delta_j^2}$$

and

$$\Gamma(E) = E - \sum_j \frac{(E - E_i)}{\Delta_j} \Omega_j(E), \quad (5)$$

*Eq. (4) reduces to the result of ref [10] for a single N environment.

The modified densities of states

the 3D and 2D densities of states can be derived

$$N_{3D}(E) = -\frac{(2m^*)^{3/2}}{4\pi^2\hbar^3} \Omega(E) \left\{ 2\left[\left[\Gamma^2(E) + \Omega^2(E) \right]^{1/2} - \Gamma(E) \right] \right\}^{-1/2} \quad (6)$$

and

$$N_{2D}(E) = \frac{m^*}{2\pi\hbar^2} \left\{ \frac{1}{2} - \frac{1}{\pi} \arctan\left(\frac{\Gamma(E)}{\Omega(E)} \right) \right\}. \quad (7)$$

In the limit as $D_j \to 0$, we have

$$\lim_{\Delta_i \to 0} N_{2D}(E) = \begin{cases} \frac{m^*}{2\pi\hbar^2}, & \gamma(E) > 0, \\ 0, & \gamma(E) < 0. \end{cases} \quad (8)$$

and

$$\lim_{\Delta_i \to 0} N_{3D}(E) = \frac{(2m^*)^{3/2}}{4\pi^2\hbar^3} \gamma^{1/2}(E). \quad (9)$$

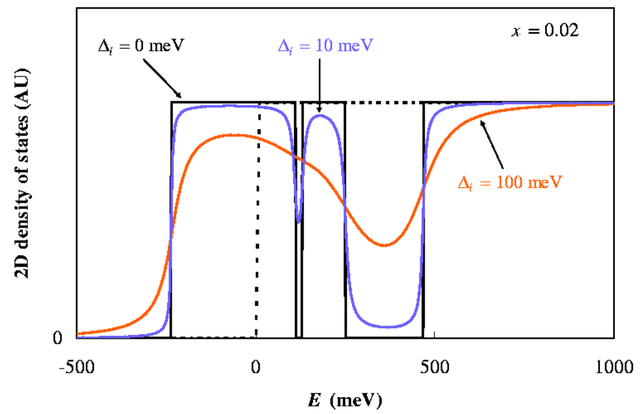

Figure 3 The 2D density of states for a 3 band model (see figure 1). The dotted line shows the density of states of the matrix semiconductor.

References (as cited in manuscript)

[1] M. Weyers, M. Sato, H. Ando, Jpn. J. Appl. Phys. Pt. 2., **31**, p. L853, (1992)

[2] W. Shan *et al*, Phys. Rev. Lett., **82**, p. 1221, (1999)

[3] B.K. Ridley, private conversation, (2003)

[4] B. K. Ridley and T. B. Watkins, Proc. Phys. Soc. London **78**, p. 293, (1961)

[5] J. B. Gunn, Solid State Commun. **1**, p. 88, (1963)

[6] A. Patane *et al*, Phys. Rev. B, **72**, p. 033312 (2005)

[7] A. Lindsay, PhD Thesis, University of Surrey, (2002)

[8] S. Fahy and E.P. O'Reilly, Physica E, **21**, p. 881 (2004)

[9] S.B. Healy, A. Lindsay and E.P. O'Reilly, IEE Proc.-Optoelectron., **151**, p. 397 (2004)

[10] J. Wu, W. Walukiewicz, E.E. Haller, Phys. Rev. B, **65**, p. 233210, (2002)

[11] P.W. Anderson, Phys. Rev., **124**, p. 41 (1961)

[12] P. Soven, Phys. Rev., **156**, p. 809 (1966)

Contact: mpvaug@essex.ac.uk