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

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Using the 2-level band anticrossing (BAC) model or its generalisation to $n$-bands, 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.

1 Introduction

It is well known that the introduction of dilute concentrations of nitrogen into III-V semiconductors causes a large red-shift of the energy gap [1]. This has been well-modelled phenomenologically by the band-anticrossing (BAC) model [2], which predicts the splitting of the conduction band around the resonant energy level of an isolated nitrogen impurity. The BAC model is often extrapolated to give the dispersion relations, predicting a profound non-parabolicity at fairly modest wavevectors. It has been suggested [3] that this may provide a mechanism for a negative differential resistance (NDR) at high fields quite different from the transferred electron effect [4, 5].

A simple model of high-field transport based on the BAC model has been derived by Patane et al. [6], who have observed an NDR effect in dilute GaNAs samples. However, in order to develop more sophisticated models, such as a hot-electron analysis, we need to perform integrals of the scattering mechanisms over $k$-space. This introduces a problem, since the density of states predicted by the BAC model is not well behaved near the nitrogen energy $E_N$. The problem is exacerbated if additional nitrogen clusters such as N-N clusters (a shared nearest neighbour Ga ion) are included. The effects of such clusters can be introduced by extending the BAC to include additional N environments [7–9]. However, since the N-N energy level can be close to the conduction band edge in GaNAs, the effects of the non-parabolicity will arise at even lower energies.

2 The dispersion relations in dilute nitrides

In the original BAC model, the energy $E$ of the band-edge in a dilute nitride material with nitrogen concentration $x$ can be found from the characteristic equation

$$
\begin{bmatrix}
E - E_M \\
\beta x^{1/2} \\
E - E_N
\end{bmatrix}
= 0,
$$

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where \( E_M \) and \( E_N \) are the energies of the matrix semiconductor and the resonant nitrogen state respectively and \( \beta \) is a measure of the interaction between the localised and extended states. This leads to a quadratic in \( E \) with the two solutions often being denoted by \( E_- \) and \( E_+ \). Additional nitrogen complexes can be incorporated by generalising to an \( n \)-band model \([7–9]\)

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

(2)

where the \( x_i \) are the concentrations of the \( i \)th type of nitrogen environment with energy \( E_i \). The dispersion relations for the dilute nitride calculated using this expression will be highly non-parabolic. In general, we can deal with the non-parabolicity by defining a function of energy

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

(3)

In the present case, it is mathematically convenient to retain the definition of \( m^* \) as the matrix semiconductor effective mass. Putting \( E_M = \hbar^2 k^2 / 2m^* \), we obtain

\[
\gamma(E) = \sum_i \frac{\beta_i^2 x_i}{E_i - E + E}.
\]

(4)

Using this formulation, the electron group velocity and band-edge effective mass can be given in terms of \( \gamma(E) \). However, if we try to formulate the densities of states using Eq. (3), we encounter a problem. The formal expressions would usually be

\[
N_{3D}(E) = \frac{(2m^*)^{3/2}}{(4\pi\hbar^3)} \gamma^{1/2}(E) d\gamma/dE \\
N_{2D}(E) = \frac{m^*}{(2\pi\hbar^2)} d\gamma/dE
\]

for the 3D and 2D densities of states respectively. Now the integrals of these expressions over energy will be proportional to \( \gamma^{3/2}(E) \) (in 3D) or \( \gamma(E) \) (in 2D). Clearly, from Eq. (4), either of these will approach infinity as \( E \) approaches any \( E_i \). This implies that there are an infinite number of states with energy less than any \( E_i \), which is physically invalid.

3 The Green’s function approach A possible solution to the problem may be provided by the approach of Wu et al. [10], who derive Eq. (1) from Anderson’s many-impurity model [11] in the coherent potential approximation [12] for the case of a single nitrogen environment. The dispersion relations can be found from the poles of the Green’s function \( G(E, E_M) \), whilst the density of states can be found by integrating the imaginary part of \( G(E, E_M) \) over \( E_M \). Analytical solutions can be found for this integral. However, we note that by generalising Wu et al.’s result, we can reproduce Eq. (2) from the poles of

\[
G(E, E_M) = \left\{ E - E_M(k) - \sum_j \frac{\beta_j^2 x_j}{E_j - E + i\Delta_j} \right\}^{-1},
\]

(5)

where the \( \Delta_j \) are interpreted as energy broadenings on the impurity levels \( E_j \). Equation (5) reduces to Wu et al.’s result in the case of a single N environment. Defining

\[
\Omega_j(E) = -\sum_k \Omega_j(E), \quad \Omega_j(E) = \frac{\beta_j^2 x_j\Delta_j}{(E - E_j)^2 + \Delta_j^2} \quad \text{and} \quad \Gamma(E) = E - \sum_j \left( \frac{E - E_j}{\Delta_j} \right) \Omega_j(E),
\]

(6)

we find that, after integrating the imaginary part of Eq. (5) over \( E_M \), the 3D and 2D densities of states are

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

(7)
and

\[ N_{3D}(E) = \frac{m^*}{2\pi\hbar} \left[ \frac{1}{2} - \frac{1}{\pi} \arctan \left( \frac{\Gamma(E)}{\Omega(E)} \right) \right]. \]  

(8)

If we now take the limit as all the broadenings \( \Delta_j \to 0 \), we find, firstly that \( \lim_{\Delta_j \to 0} \Gamma(E) = \gamma(E) \), so, for the 3D density of states we have

\[ \lim_{\Delta_j \to 0} N_{3D}(E) = \frac{(2m^*)^{3/2}}{4\pi^2\hbar^3} \gamma^{3/2}(E). \]  

(9)

This is almost in the conventional form for the density of states except that the derivative of \( \gamma(E) \) is no longer included. Whilst this still tends to infinity near the resonant energy levels, we find that its integral over energy does converge. This is more clearly seen in the 2D case. By considering the behaviour of the quotient \( \Gamma(E)/\Omega(E) \) near the band-edge energies (where \( \gamma(E) = 0 \)) and the N complex energies, we find

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

(10)

Note that the non-zero value is the same as for the matrix semiconductor. Only the energy range over which it is non-zero changes. In the case of a single isolated nitrogen impurity, it is easy to show that the gap between \( E_N \) and the bottom of \( E_+ \) is the same as the downward shift in \( E_- \). Hence, the number of states less than the edge of \( E_+ \) is the same in the dilute nitride as in the matrix semiconductor.

In conclusion, we have found that by adopting a Green’s function approach, we can derive analytical functions for the 2D and 3D densities of states that remain well-behaved around the nitrogen complex energy levels and conserve the number of states. This gives us a consistent mathematical starting point from which we may proceed with high field calculations.

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References