Electron transport in dilute nitrides

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Overview

• Effects of non-parabolicity
  – Problem with the density of states
• Observed mobilities
• Models of alloy / nitrogen scattering
• Solution of the Boltzmann equation
  – The ‘ladder method’
  – Calculations
• Conclusions
Non-parabolicity

Band anticrossing (BAC) model\(^1\)

- Effective mass
- Density of states
- Group velocity

General formula for dispersion relations

The dispersion relations can be written in the form:

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

where

\[ \gamma(E) = \frac{\beta^2 x}{E_N - E} + E - E_c, \]

(From BAC model\(^1\)).

Densities of states (DOS) in non-parabolic bands

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

3D density of states.

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

2D density of states.

However...
The density of states

- Becomes infinite at $E_N$
- Predicts infinite number of states below $E_N$
The Green’s function approach

Wu et al\textsuperscript{1} find Green’s function from Anderson many-impurity model\textsuperscript{2}

\begin{equation}
G(E, E_M) = \left\{ E - E_M - \frac{\beta^2 x}{E - E_N + i\Delta} \right\}^{-1}.
\end{equation}

Density of states is then

\begin{equation}
N(E) = -\frac{1}{\pi} \text{Im} \int G(E, E_M) N_0(E_M) dE_M.
\end{equation}

where $N_0$ is the DOS in matrix semiconductor.

The 3D density of states

\[ \Delta = 0 \text{ meV} \]

\[ x = 0.02 \]

\[ \Delta = 100 \text{ meV} \]
The 2D density of states

\[ \Delta = 0 \text{ meV} \]
\[ x = 0.02 \]
\[ \Delta = 100 \text{ meV} \]
The energy broadening $\Delta$

Finite $\Delta$
- interpreted as an energy broadening

$\Delta \rightarrow 0$
- factor of $d\gamma(E)/dE$ disappears from densities of states
- Predicts finite number of states below $E_N$

$\Delta \rightarrow \infty$
- densities of states approach those of the matrix semiconductor
- real part of dispersion relations become those of the matrix semiconductor
Densities of states for $\Delta \rightarrow 0$

$$N_{3D}(E) = \frac{(2m^*)^{3/2}}{4\pi^2 \hbar^3} \gamma^{1/2}(E), \quad \text{3D density of states.}$$

$$N_{2D}(E) = \frac{m^*}{2\pi \hbar^2}, \quad \text{2D density of states (within the band)}$$

$(m^*$ is the effective mass of the matrix semiconductor).

i.e. these are the same as before except that the factor of $d\gamma(E)/dE$ has disappeared.
Consequences for scattering rates and relaxation times

\[ W(E) = \frac{1}{\tau(E)} = \frac{2\pi}{\Box} |M(E)|^2 N(E), \]

Assuming \( M(E) \) is slowly varying:

- \( \tau(E) \to 0 \) as \( E \to E_N \) in 3D case but not in 2D case for modified DOS
- \( \tau(E) \to 0 \) as \( E \to E_N \) in both cases for usual DOS in non-parabolic band
- Immobility of N state manifests through group velocity.
Observed mobilities - GaInNAs 2% N (Kurtz et al\textsuperscript{1})

- Thermally activated mobility
- Activation energy decreases with increasing electron concentration
- Low $T$ mobility still large for hopping conductivity

Observed mobilities - GaNAs/AlGaaS heterostructures (Mouillet et al\textsuperscript{1})

Alloy scattering – the microscopic approach

- Alloy treated in the virtual crystal approximation
- Scattering due to fluctuations $\Delta V$ around average potential
- Nature of $\Delta V$?
  - Band-edge difference
  - Electron affinity difference
  - Electro-negativity difference
  - Dielectric approach (used to explain optical bowing in alloys)

Strain scattering?

- Strain shifts band-edge – related via deformation potential $\Xi$
- In $\Gamma$ valley energy change is through pure dilation $\Delta$
- Looking for an $r$ dependent dilation that could yield a scattering cross-section
Trial model

- Consider isolated impurity
- Assume matrix material is isotropic
- Use linear theory of elasticity in spherical polar coordinates

But...

In spherical polar coordinates, without a body force the dilation is a constant (taken to be due to external pressure) – no effect!
Alloy scattering – the phenomenological approach

• Scattering related to variation of band-edge with alloying
• Large bowing in dilute nitrides

• Hellman-Feynman theorem\textsuperscript{1}
• S-matrix theory\textsuperscript{2}

\textsuperscript{1} M. Auslender and S. Hava, \textit{Solid State Commun.}, \textbf{87}, 335 (1993)
Alloy scattering – temperature dependence

- All models predict a mobility that varies as $T^{-1/2}$
- Observed mobilities show increasing $T$ dependence at low $T$
- Low $T$ mobility possibly due to defects
Polar optical phonons – the ladder method\textsuperscript{1,2}

- Inelastic process
- Scattering rate at $E$ related to rates at $E \pm \hbar \omega$
- No unique relaxation time

Calculated relaxation times for non-parabolic bands

- \( T = 300 \) K
- Bulk GaNAs
- Normal non-parabolic DOS

Calculated mobilities\textsuperscript{1} – all processes

\[ N_D = 10^{17} \text{ cm}^2 \]
\[ N_A / N_D = 0.5 \]

\[ \lambda = 0.02 \]

Calculated mobilities\textsuperscript{1} – T dependence

Calculated mobilities\textsuperscript{1} – x dependence

$T = 300$ K

Conclusions

- High temperature mobility limited by nitrogen scattering
- Polar optical phonon scattering still important at high temperature
- Alloy scattering does not model low temperature mobility
- Low temperature mobility likely to be limited by defects / trapping centres
- For high field, effect of DOS may be significant for hot electrons
Thank you for your attention