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Electron transport in dilute nitrides

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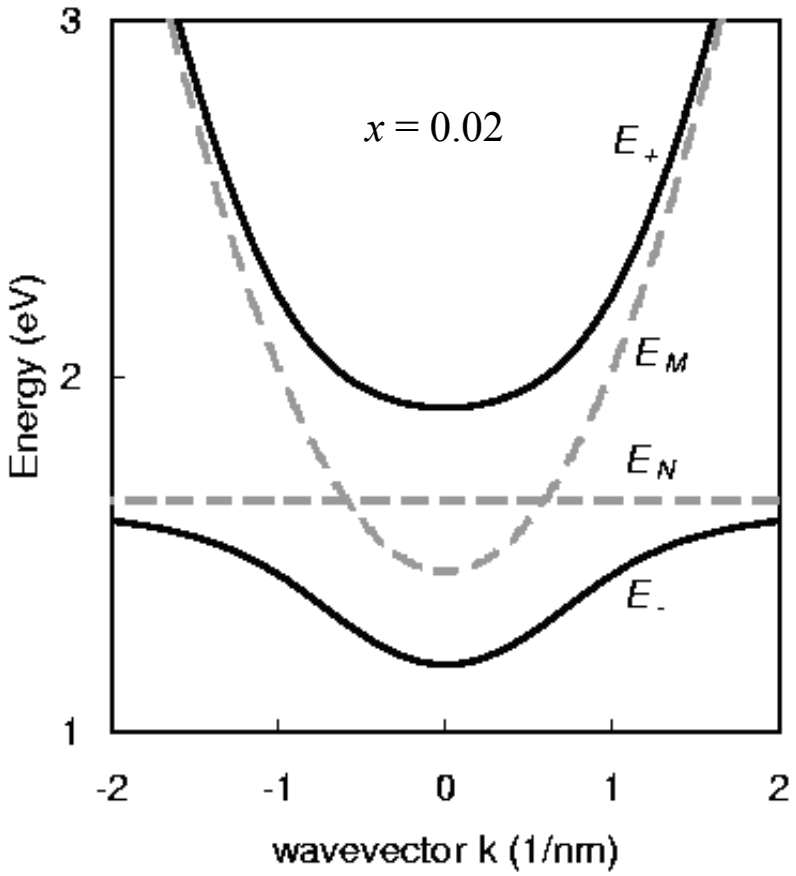
Overview

- 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

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

General formula for dispersion relations

The dispersion relations can be written in the form:

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

where

$$\gamma(E) = \frac{\beta^2 x}{E_N - E} + E - E_C,$$

(From BAC model[1]).

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

Densities of states (DOS) in non-parabolic bands

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

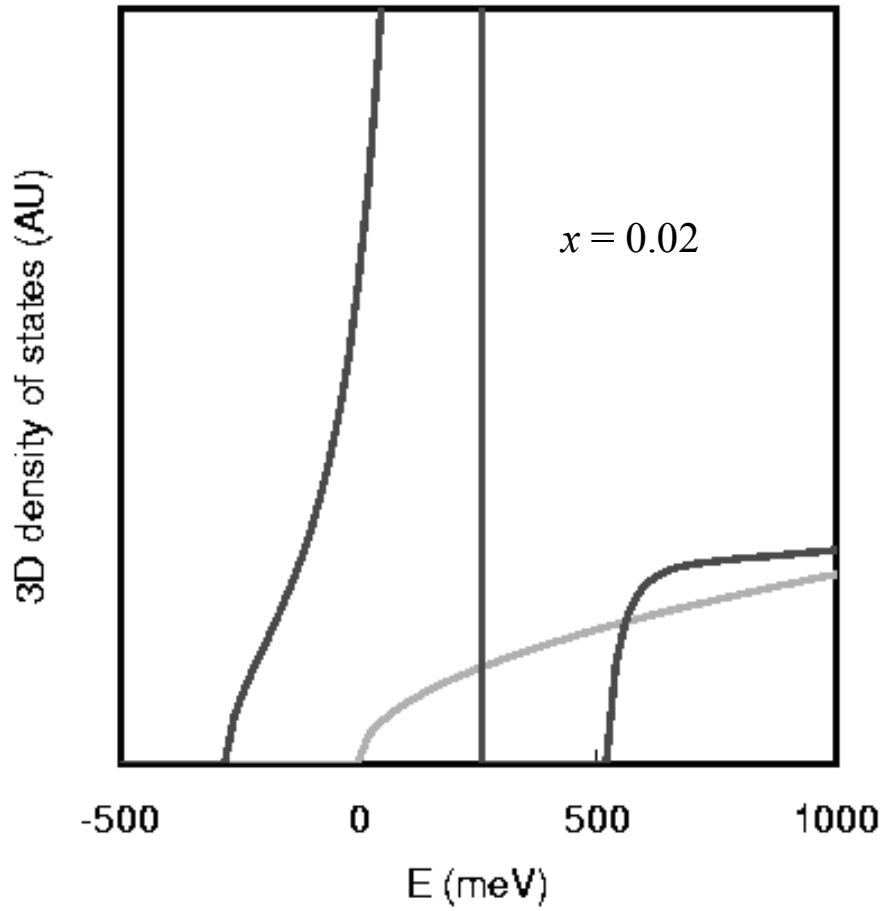
3D density of states.

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

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*[1] find Green's function from Anderson many-impurity model[2]

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

Density of states is then

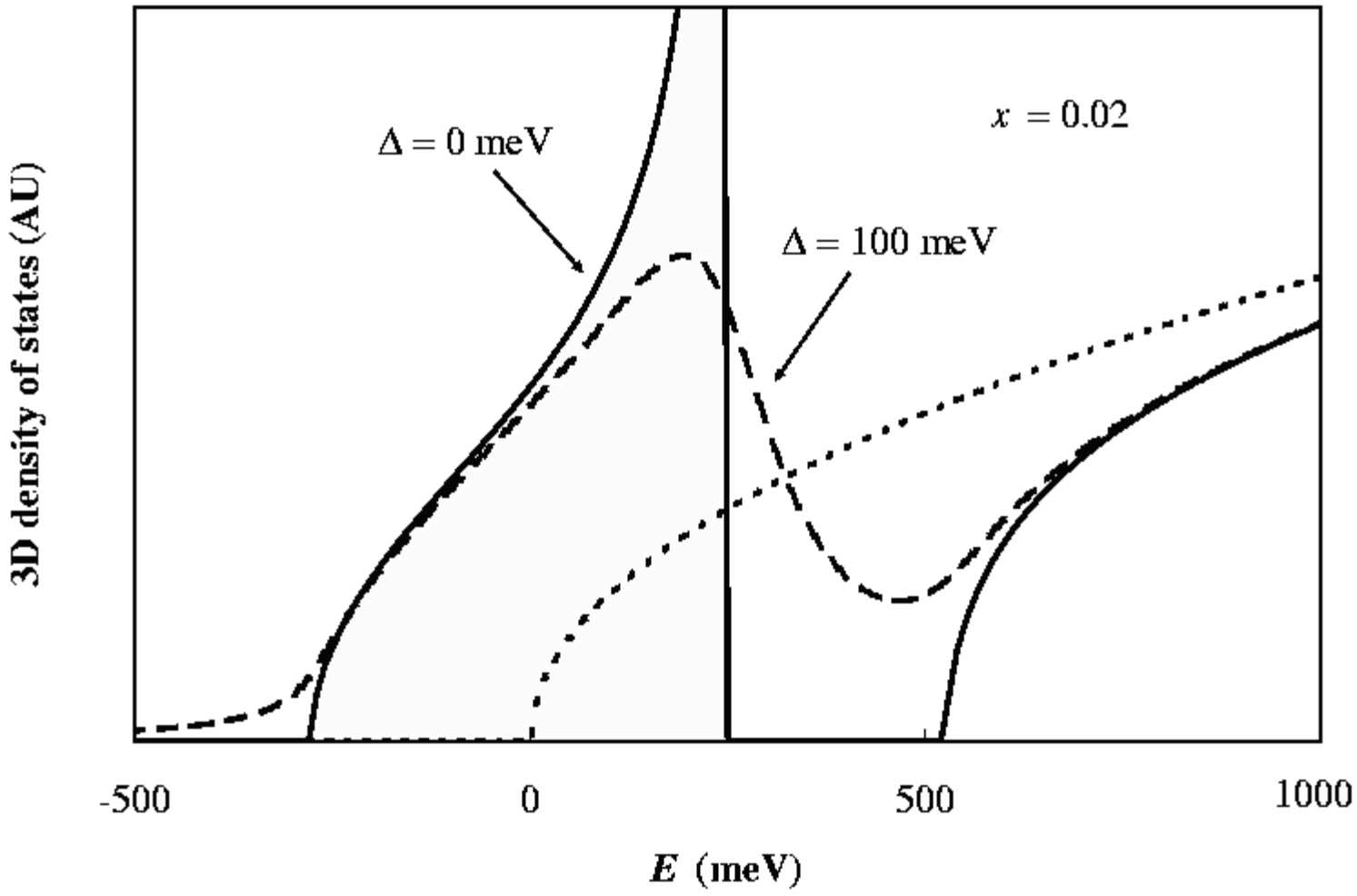
$$N\left(E\right)=-\frac{1}{\pi}\,\mathrm{Im}\int G\left(E,E_M\right)N_0\left(E_M\right)dE_M.$$

where N_0 is the DOS in matrix semiconductor.

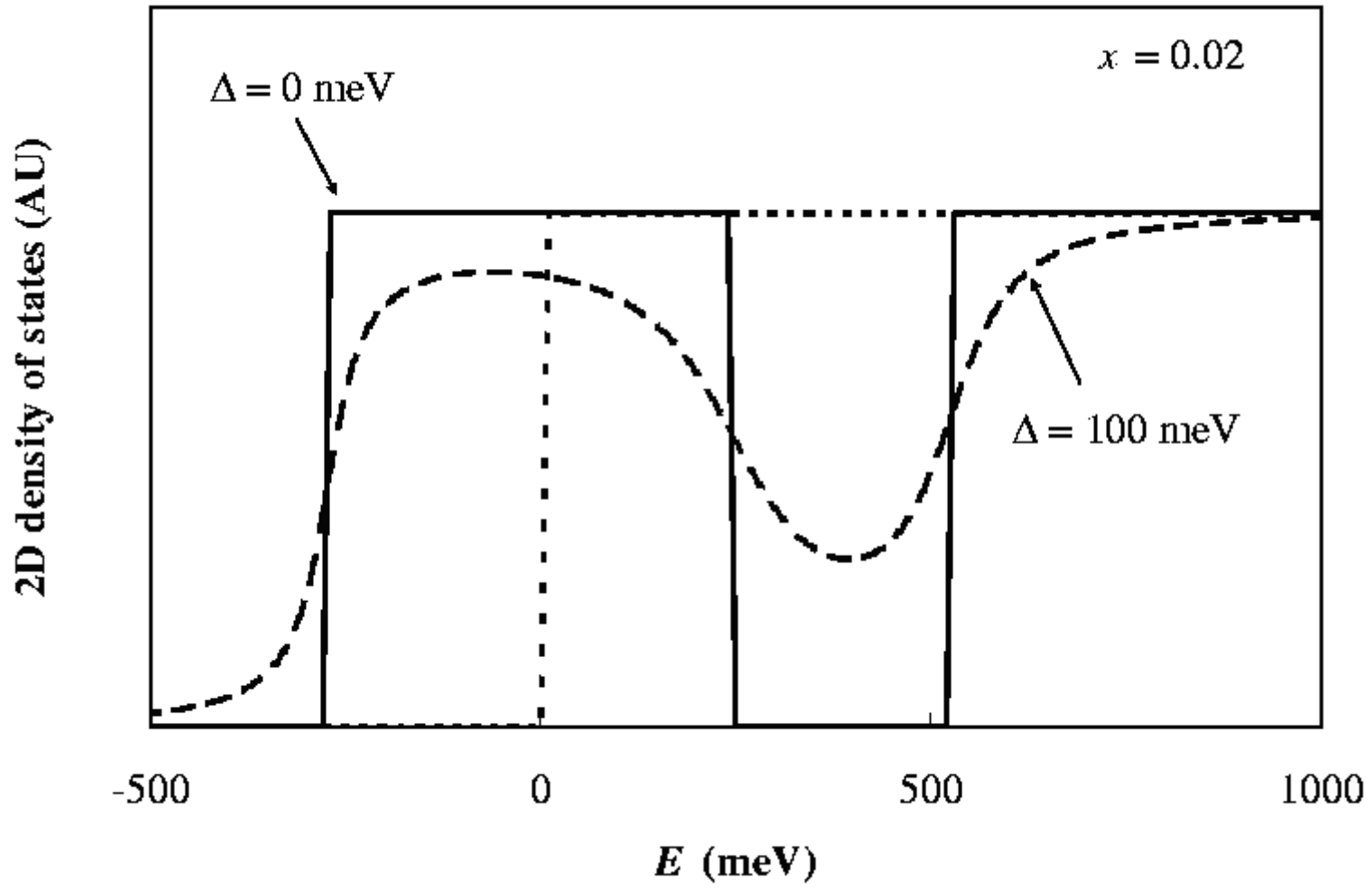
[1] J. Wu, et al, *Phys. Rev. B*, **65**, 233210, (2002)

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

The 3D density of states



The 2D density of states



The energy broadening Δ

Finite Δ

- 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 $\Delta \to 0$

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

3D density of states.

$$N_{2D}(E) = \frac{m^*}{2\pi\hbar^2},$$

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.

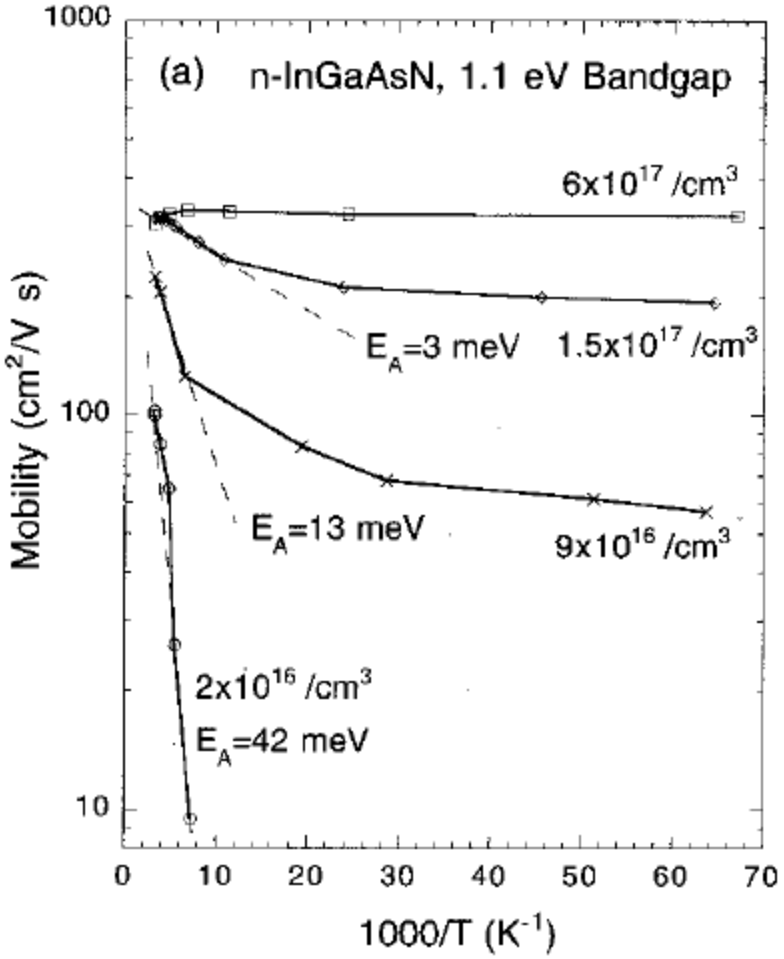
Consequences for scattering rates and relaxation times

$$W(E) = \frac{1}{\tau(E)} = \frac{2\pi}{\square}\left|M(E)\right|^2 N(E),$$

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.

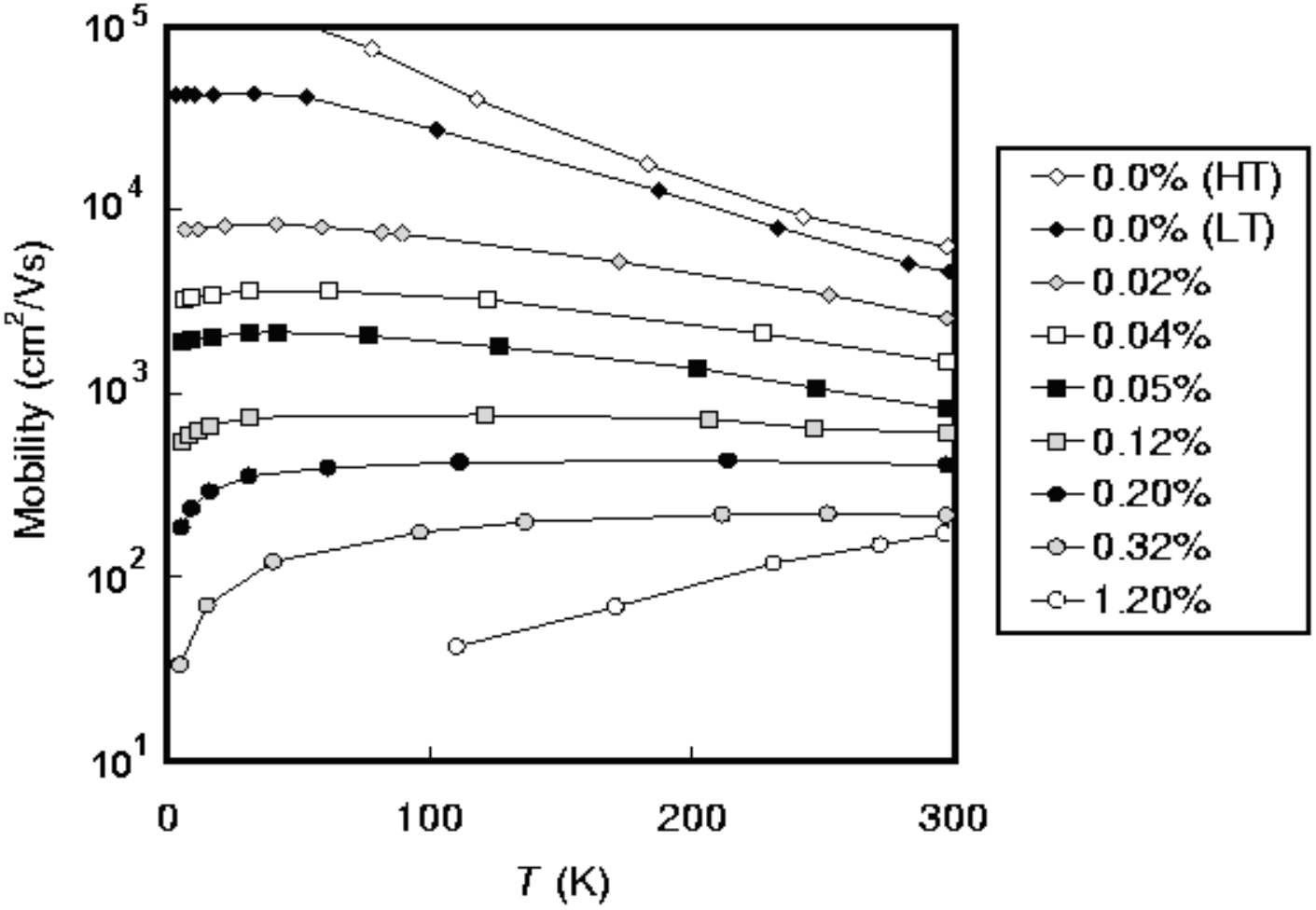
Observed mobilities - GaInNAs 2% N (Kurtz et al[1])



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

[1] Kurtz et al, *Appl. Phys. Lett*. **77**, 400 (2000)

Observed mobilities - GaNAs/AlGas heterostructures (Mouillet et al[1])



[1] R. Mouillet et al, *Solid State Commun.*, **126**, 333 (2003)

Alloy scattering – the microscopic approach[1]

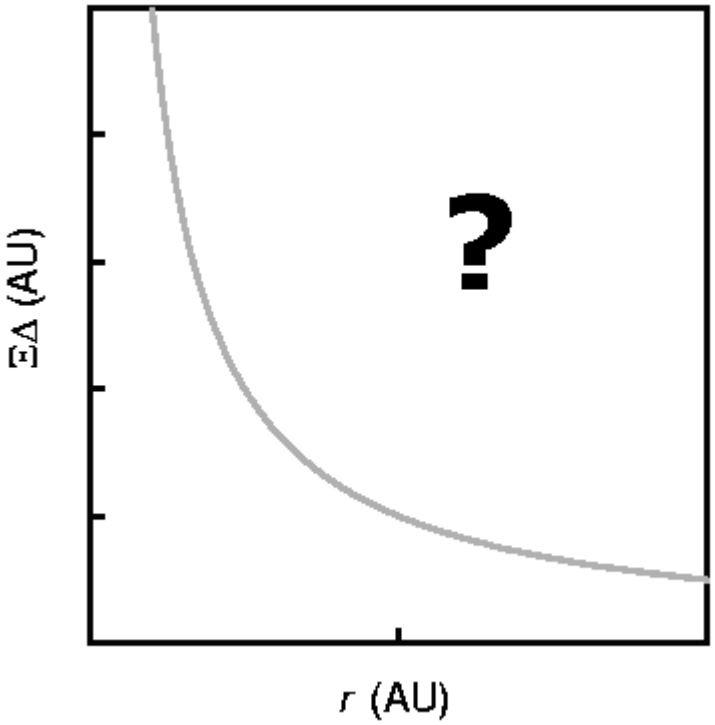
- Alloy treated in the virtual crystal approximation
- Scattering due to fluctuations ΔV around average potential
- Nature of ΔV?

  - Band-edge difference
  - Electron affinity difference
  - Electro-negativity difference
  - Dielectric approach[2] (used to explain optical bowing in alloys)

[1] J.W. Harrison and J.R. Hauser, *Phys. Rev. B*, **13**, 5347 (1976)

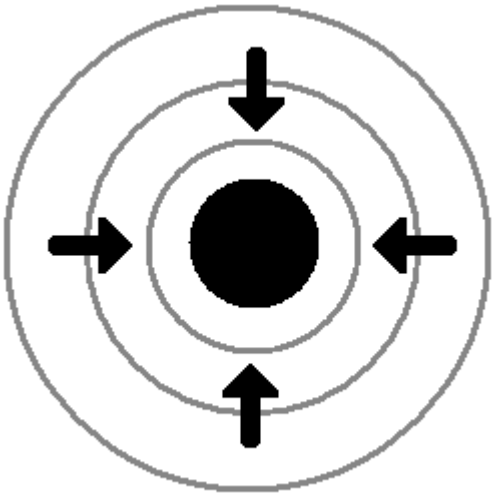
[2] J.A. Van Vechten and T.K. Bergstresser, *Phys. Rev. B*, **1**, 3351 (1970)

Strain scattering?



- Strain shifts band-edge – related via deformation potential Ξ
- In Γ valley energy change is through pure dilation Δ
- 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

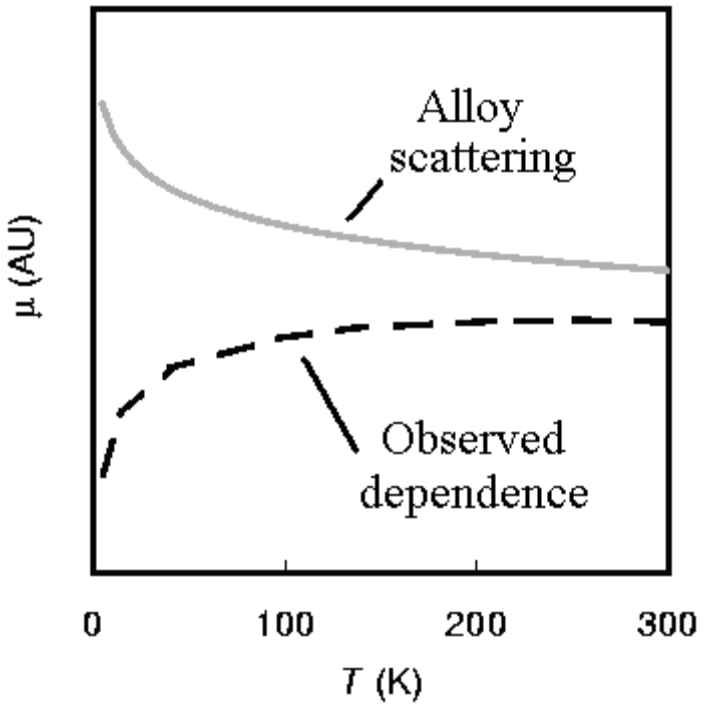
- Scattering related to variation of band-edge with alloying
- Large bowing in dilute nitrides

  - Hellman-Feynman theorem[1]
  - S-matrix theory[2]

[1] M. Auslender and S. Hava, *Solid State Commun*., **87**, 335 (1993)

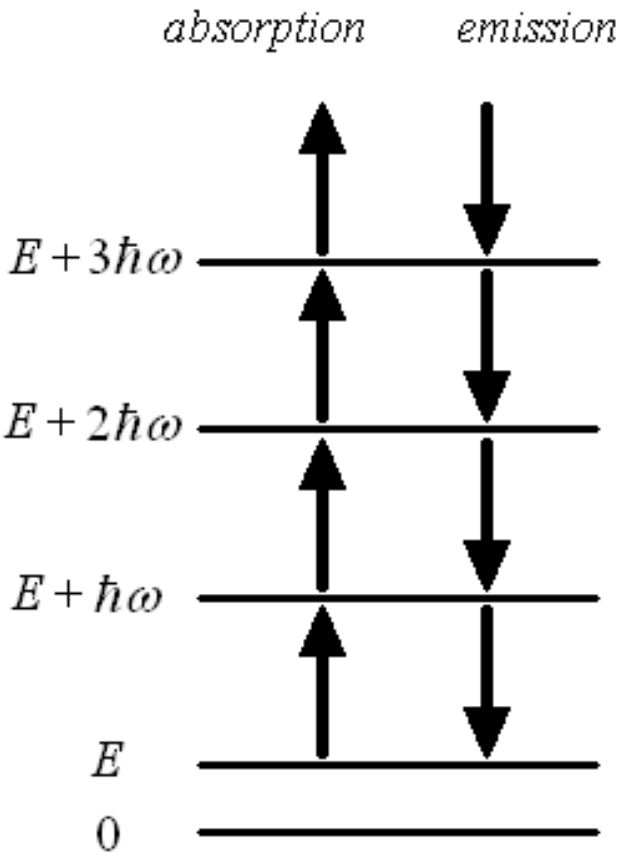
[2] S. Fahy and E.P. O'Reilly, *Appl. Phys. Lett*, **83**, 3731 (2003)

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[1,2]

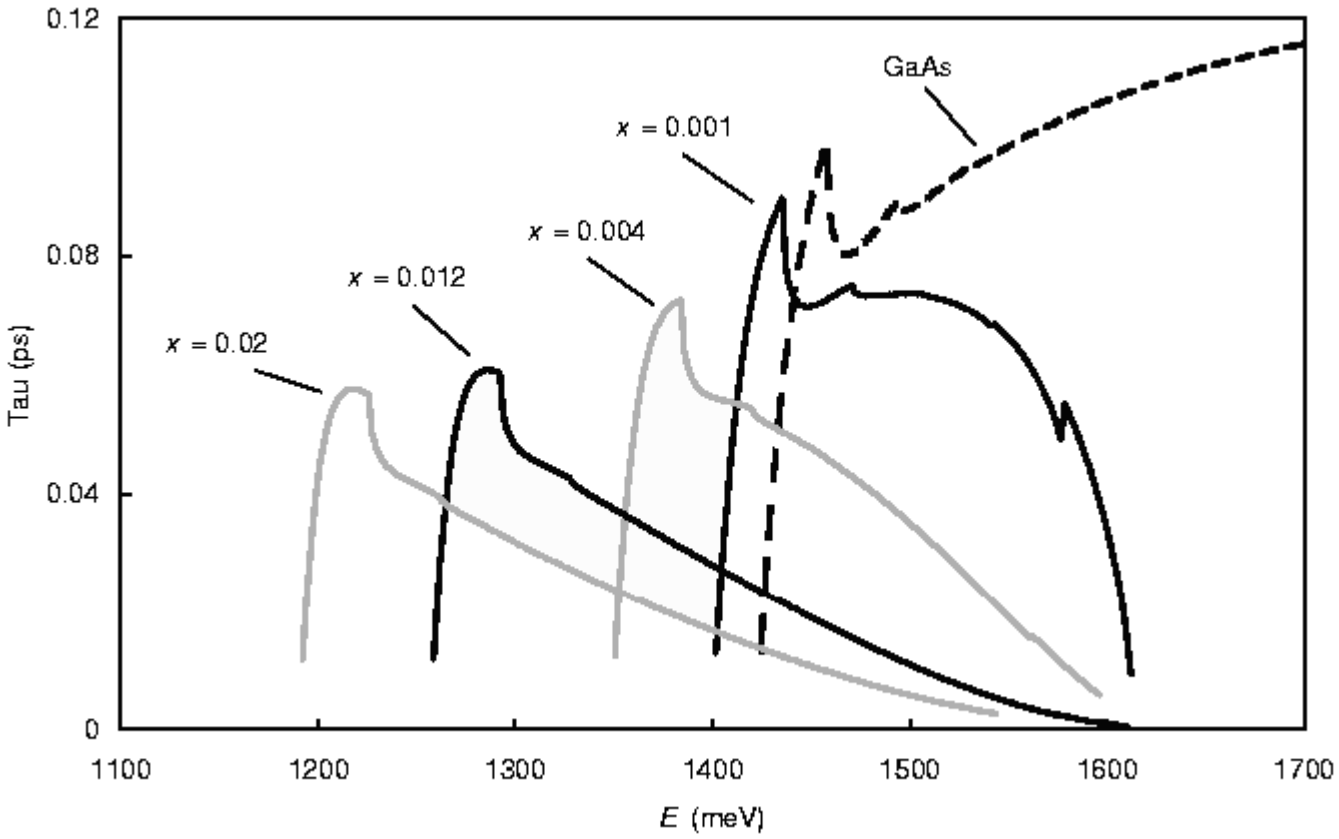


- Inelastic process
- Scattering rate at E related to rates at $E \pm \hbar w$
- No unique relaxation time

[1] R.T. Delves, *Proc. Phys. Soc.*, **73**, 572 (1959)

[2] K. Fletcher and P.N. Butcher, *J. Phys. C: Solid State Phys.*, **5**, 212 (1972)

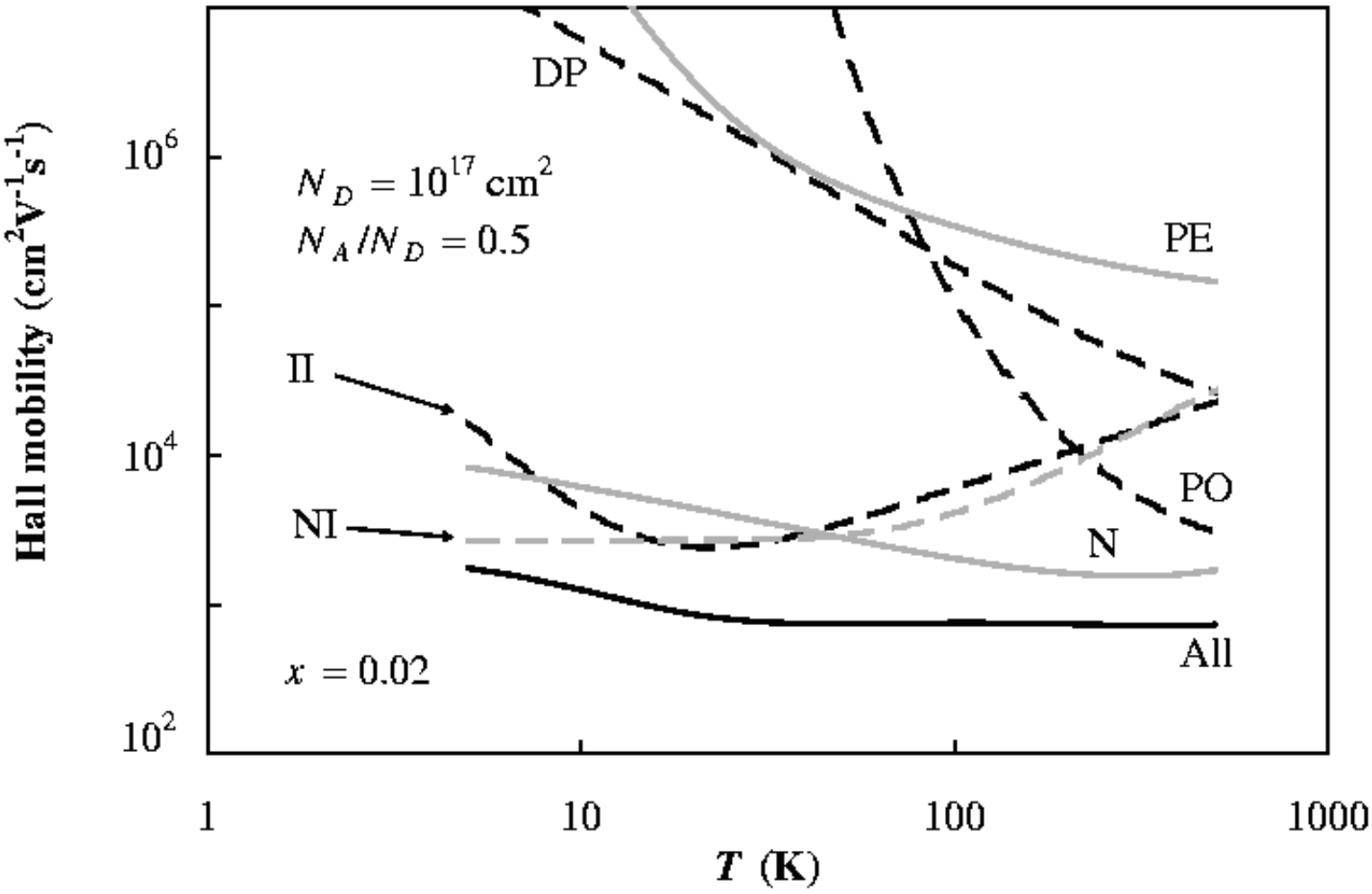
Calculated relaxation times for non-parabolic bands[1]



- T = 300 K
- Bulk GaNAs
- Normal non-parabolic DOS

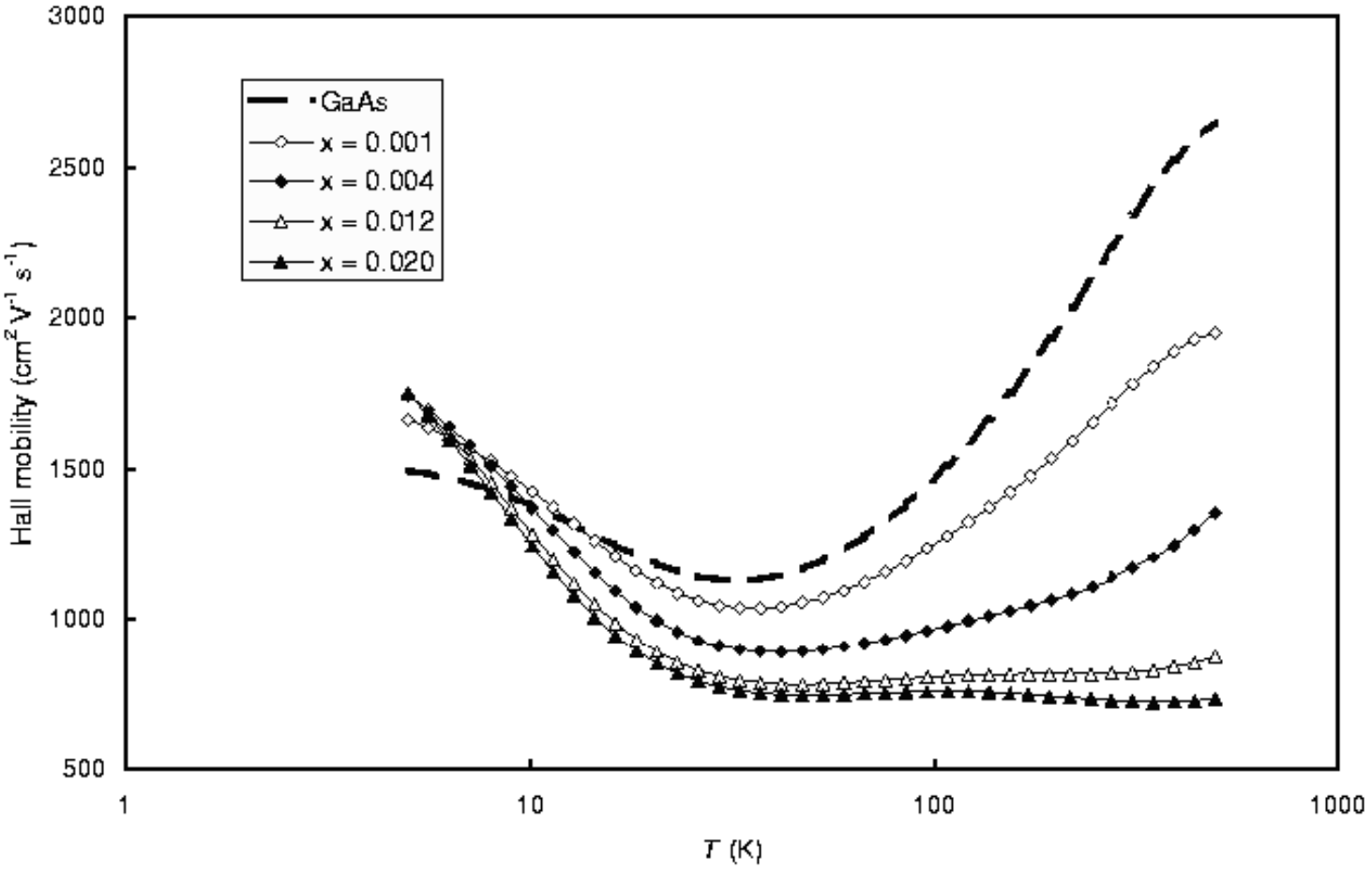
[1] M.P. Vaughan and B.K. Ridley, *Phys. Rev. B*, **72**, 075211 (2005)

Calculated mobilities[1] – all processes



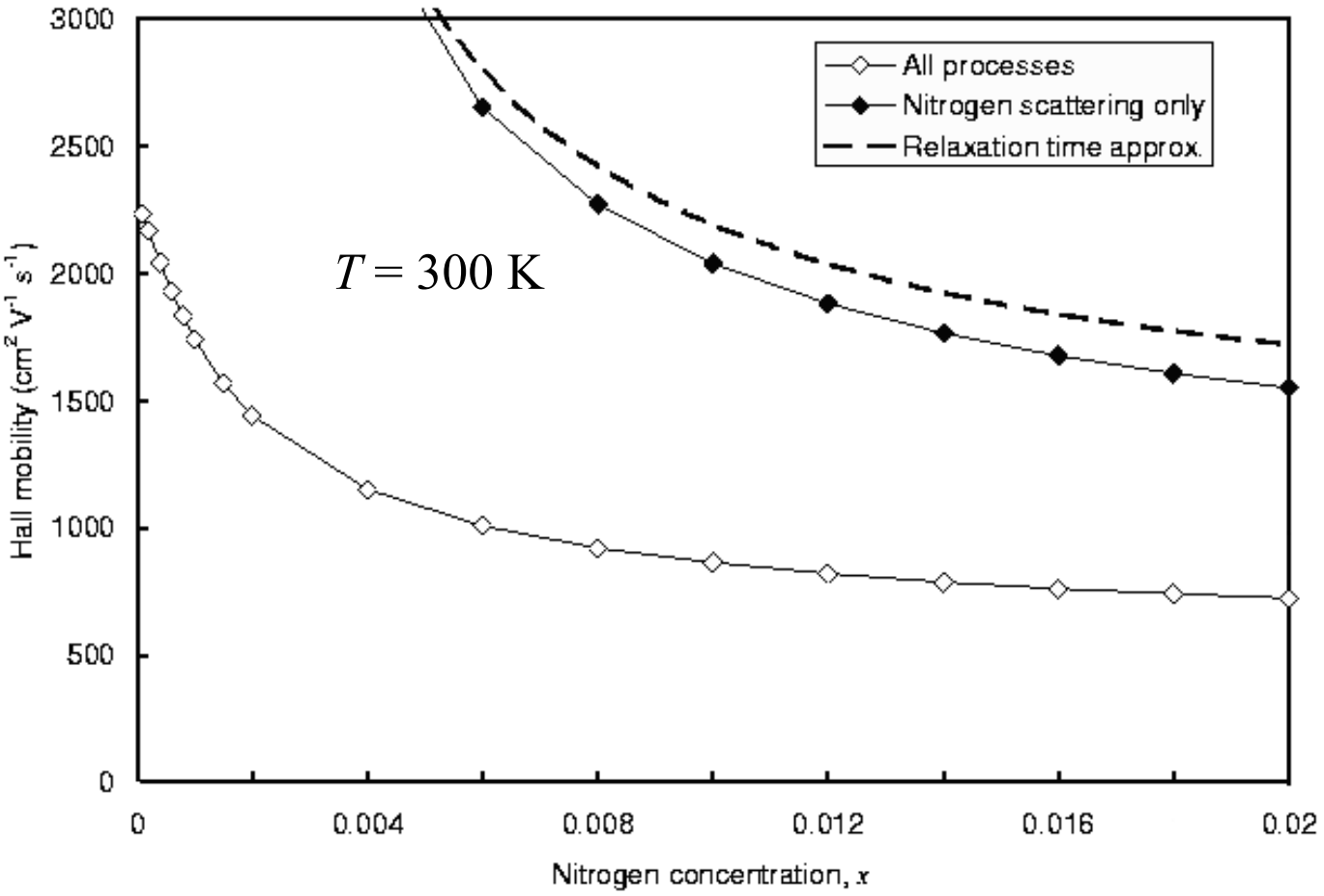
[1] M.P. Vaughan and B.K. Ridley, *Phys. Rev. B*, **72**, 075211 (2005)

Calculated mobilities[1] – T dependence



[1] M.P. Vaughan and B.K. Ridley, *Phys. Rev. B*, **72**, 075211 (2005)

Calculated mobilities[1] – x dependence



[1] M.P. Vaughan and B.K. Ridley, *Phys. Rev. B*, **72**, 075211 (2005)

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

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