Experimental determination and theoretical modelling of the density of states in GaNAs

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Overview

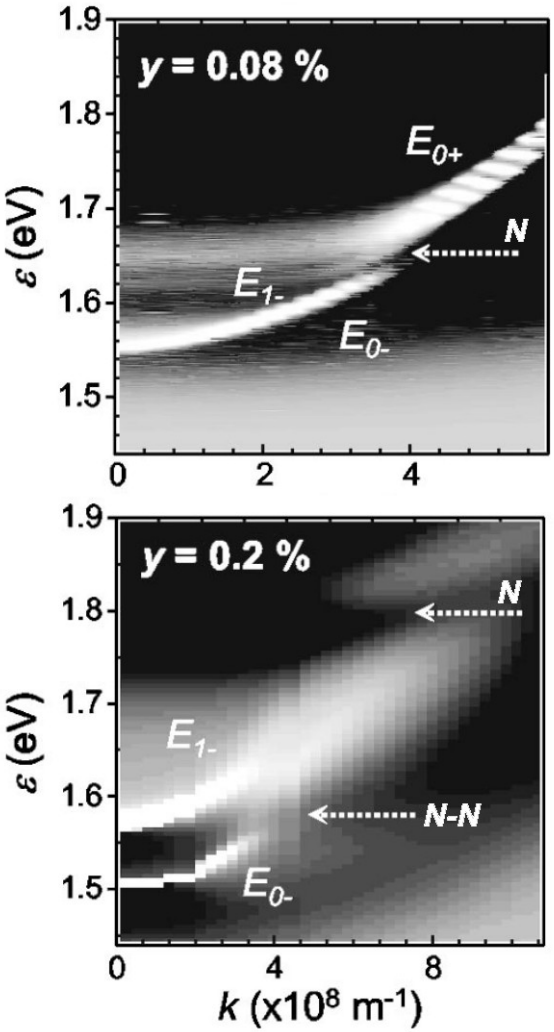
- Motivation
- Measuring the Density of States (DOS) via Scanning Tunnelling Spectroscopy (STS)
  - Theory
- Green's function approach to density of states
- Linear Combination of Isolated Nitrogen States (LCINS) model
- Intrinsic broadening
  - Homogeneous and inhomogeneous
- Extrinsic broadening effects
  - Thermal
  - Modulation sampling
- Results and discussion

Motivation

Despite many years of research into dilute nitrides, the DOS has never been determined experimentally way from the CBE.

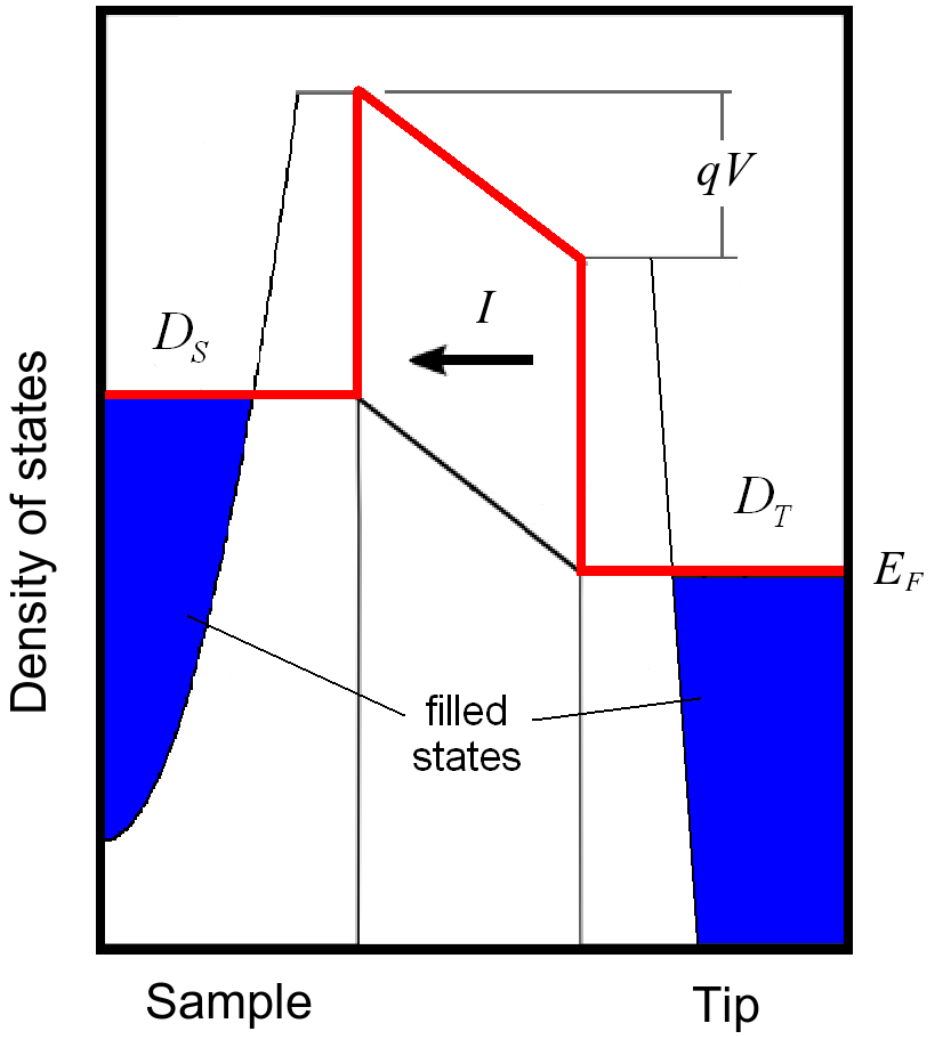
Magneto-tunnelling measurements have been conducted for ultra-dilute samples by **Patanè** *et al* [1] (right), showing the break up of the band near N and N-N pair cluster states.

- The present work represents the first determination of the DOS in GaNAs away from band-edge
- Beyond ultra-dilute range (1.2% nitrogen)
- Important for applications such as APDS



Images from Ref. [1]

[1] A Patanè *et al*, *Phys. Rev. B,* **71**, 195307 (2005).



Assuming the tip density of states D_T **is constant**, then in the limit $T \to 0$, the **differential conductance** is

$$\lim_{k_B T \to 0} \frac{dI}{dV} = \frac{4\pi q^2}{\hbar} D_T |M|^2 D_S(E_F - qV)$$

D_S is the sample **local density of states.**

(M is the transmission matrix)

The Green's function of the system is found to be [2]

$$G(E,E_{\mathbf{k}}) = \left\{ E - E_{\mathbf{k}} - \frac{1}{N_C} \sum_{\mathbf{j}} \frac{V_{\mathbf{j}}^2}{E - E_{\mathbf{j}} + i\Delta_{\mathbf{j}}} \right\}^{-1}$$

$E_{\mathbf{k}}$ - unperturbed extended state energies,

$E_{\mathbf{j}}$ - N state energies (**required parameters**),

$V_{\mathbf{j}}$ - interaction energies (**required parameters**),

$\Delta_{\mathbf{j}}$ – homogeneous energy broadenings (**predicted by model**).

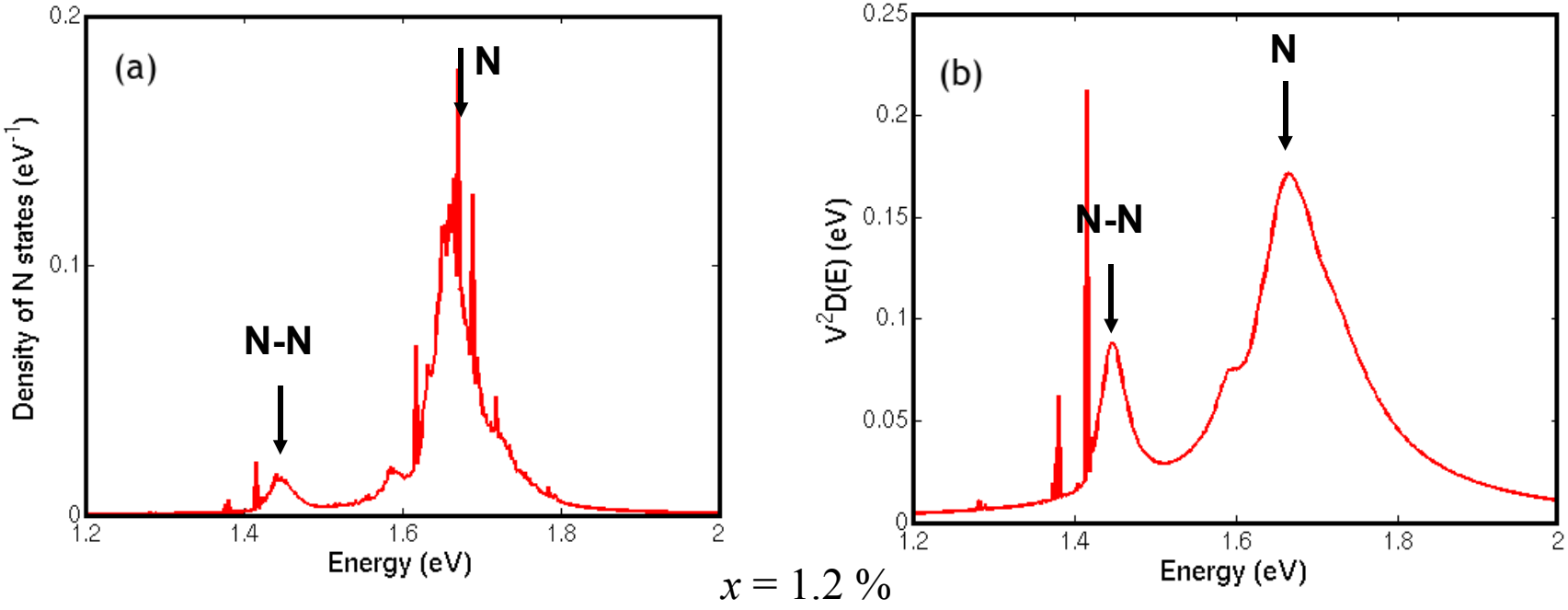
The DOS projected on to the **k**-states is then

$$D(E) = -\frac{1}{\pi} \mathrm{Im} \int G(E,E_{\mathbf{k}}) D_0(E_{\mathbf{k}}) dE_{\mathbf{k}}$$

$D_0(E)$ - density of states of the unperturbed system.

[2] M.P. Vaughan and B. K. Ridley, *Phys. Rev. B,* **75**, 195205 (2007)

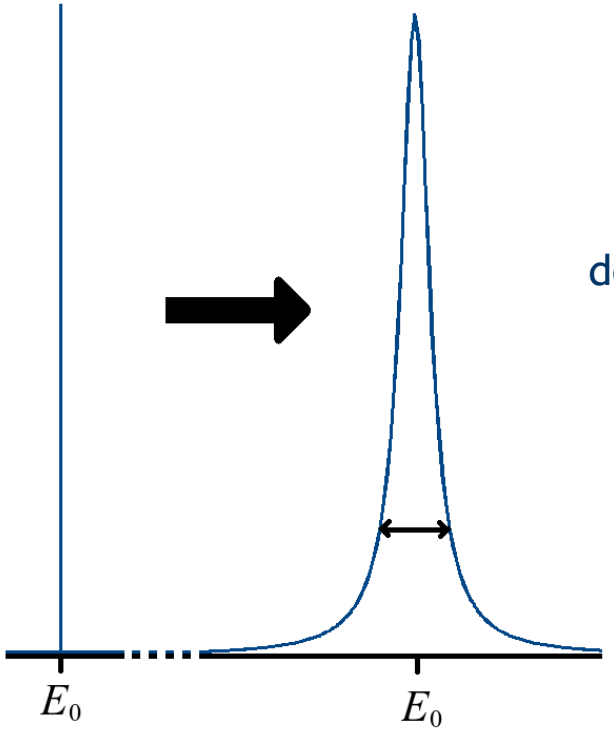
Linear Combination of Isolated Nitrogen States (LCINS)



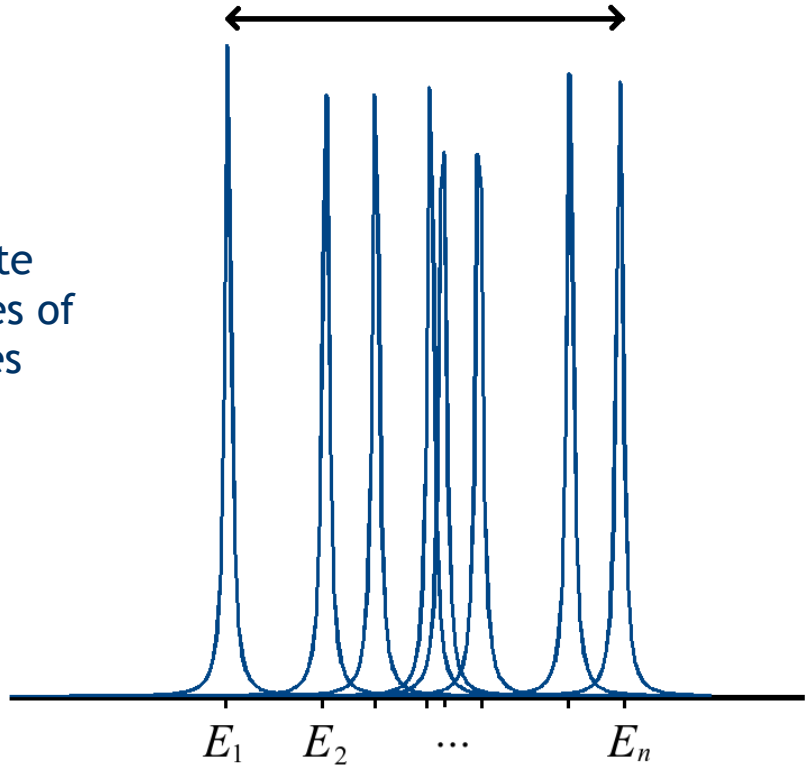
$x = 1.2\ \%$

- N – state energies E_j and interaction energies V_j extracted from full tight binding calculations [3]
- Results may be used directly with the Green's function formulation

[3] A. Lindsay and E.P. O'Reilly, *Phys. Rev. Lett.*, **93**, 196402 (2004)



N state densities of states



Homogeneous or 'lifetime' broadening

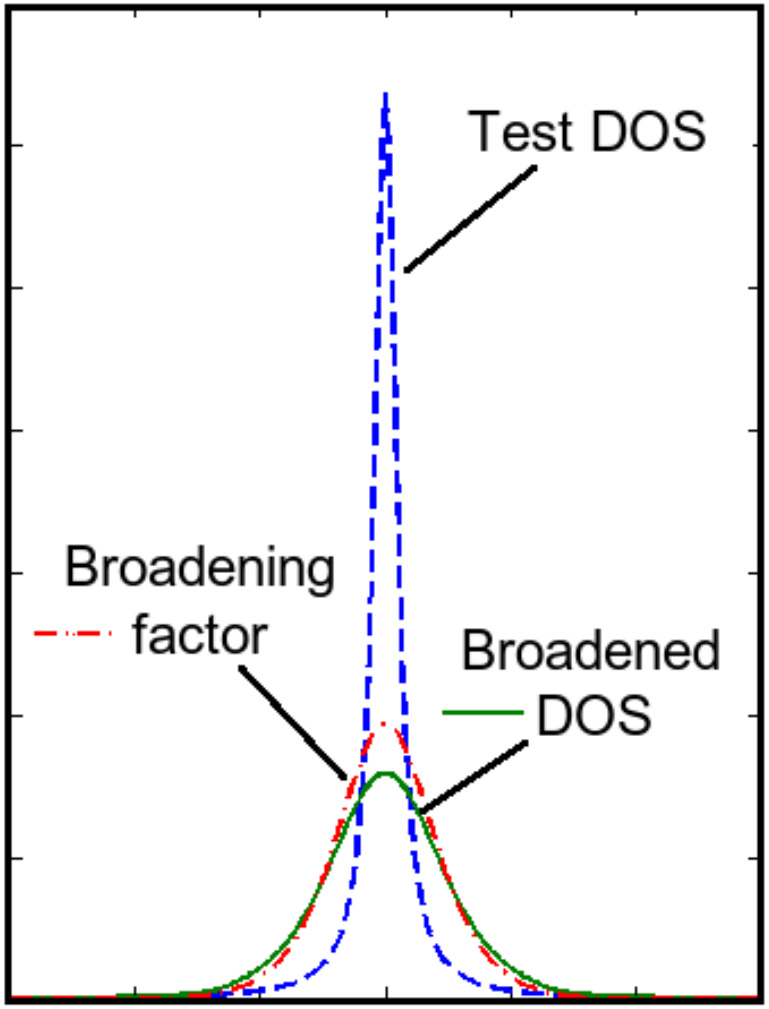
$$\delta(E-E_0) \rightarrow \frac{1}{\pi}\frac{(\Delta/2)}{(E-E_0)^2+(\Delta/2)^2}$$

Intrinsic to Green's function approach

Inhomogeneous broadening – many states distributed in energy.

Not intrinsic to Green's function approach

Natural feature of LCINS model

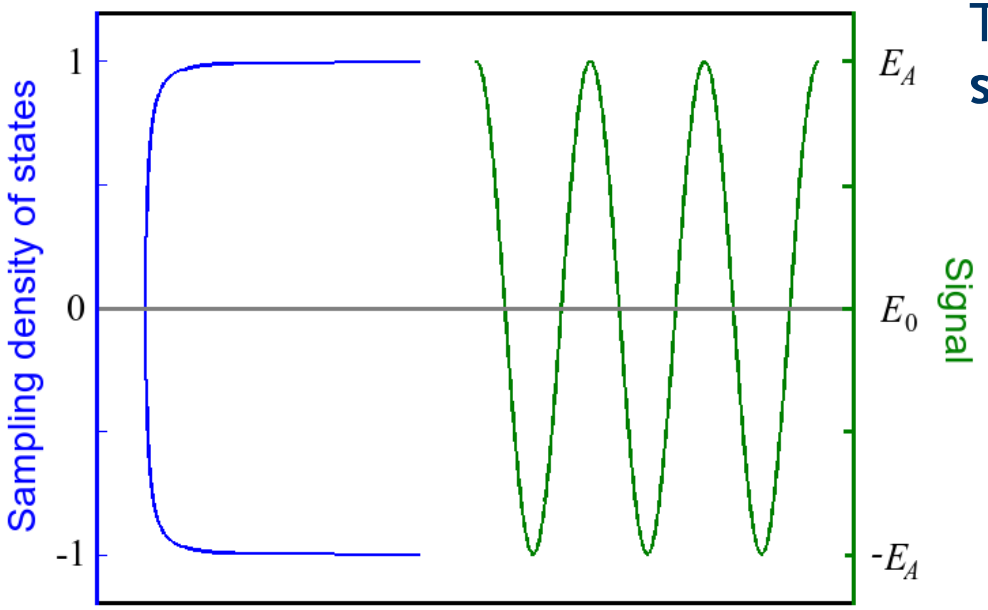


For $T \neq 0$, the differential conductance is

$$\frac{dI}{dV} = \frac{4\pi q^2}{\hbar} D_T |M|^2 \times \int_{-\infty}^{\infty} \frac{1}{k_B T} \frac{e^{\varepsilon / k_B T}}{\left(1 + e^{\varepsilon / k_B T}\right)^2} D_S\left(E_F - qV + \varepsilon\right) d\varepsilon$$

Broadening factor (derivative of Fermi-Dirac factor)

Graph shows test Lorentzian (FWHM 20 meV) thermally broadened at $T = 300$ K

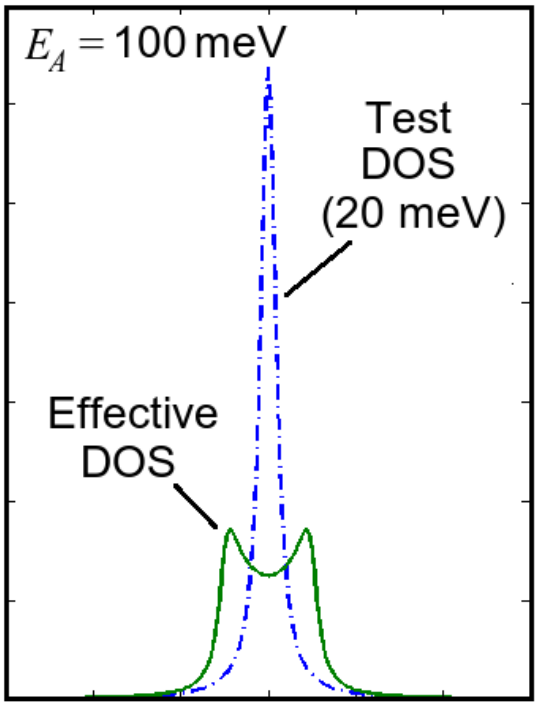


Modulation of the voltage gives rise a **sampling density of states**

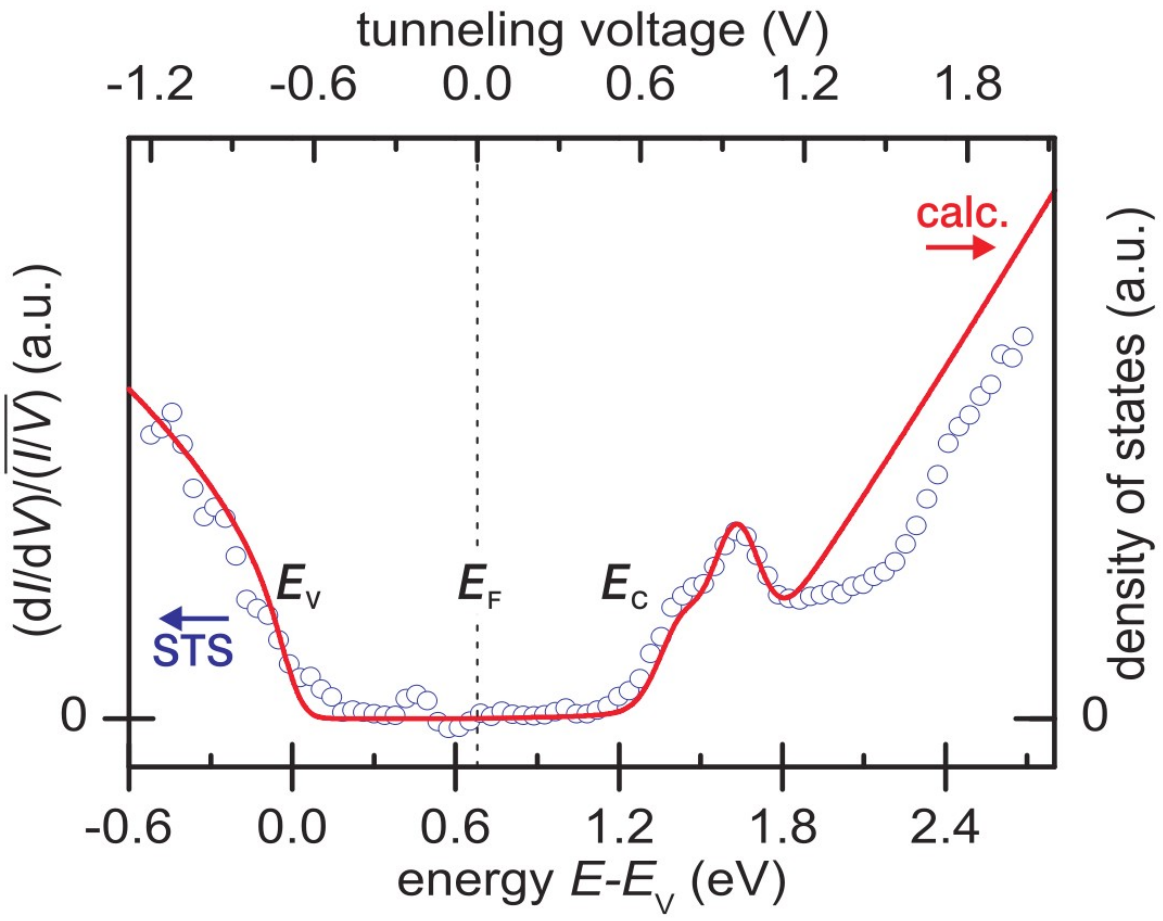
$$D_m(E,E_0)=\frac{1}{\pi E_A}\left(1-\left[\frac{E-E_0}{E_A}\right]^2\right)^{-1/2}$$

This gives an **effective density of states**

$$D_S(E)\rightarrow\int_{E-E_A}^{E+E_A}D_m(E',E)D_S(E')\,dE'$$



Results - valence and conduction bands

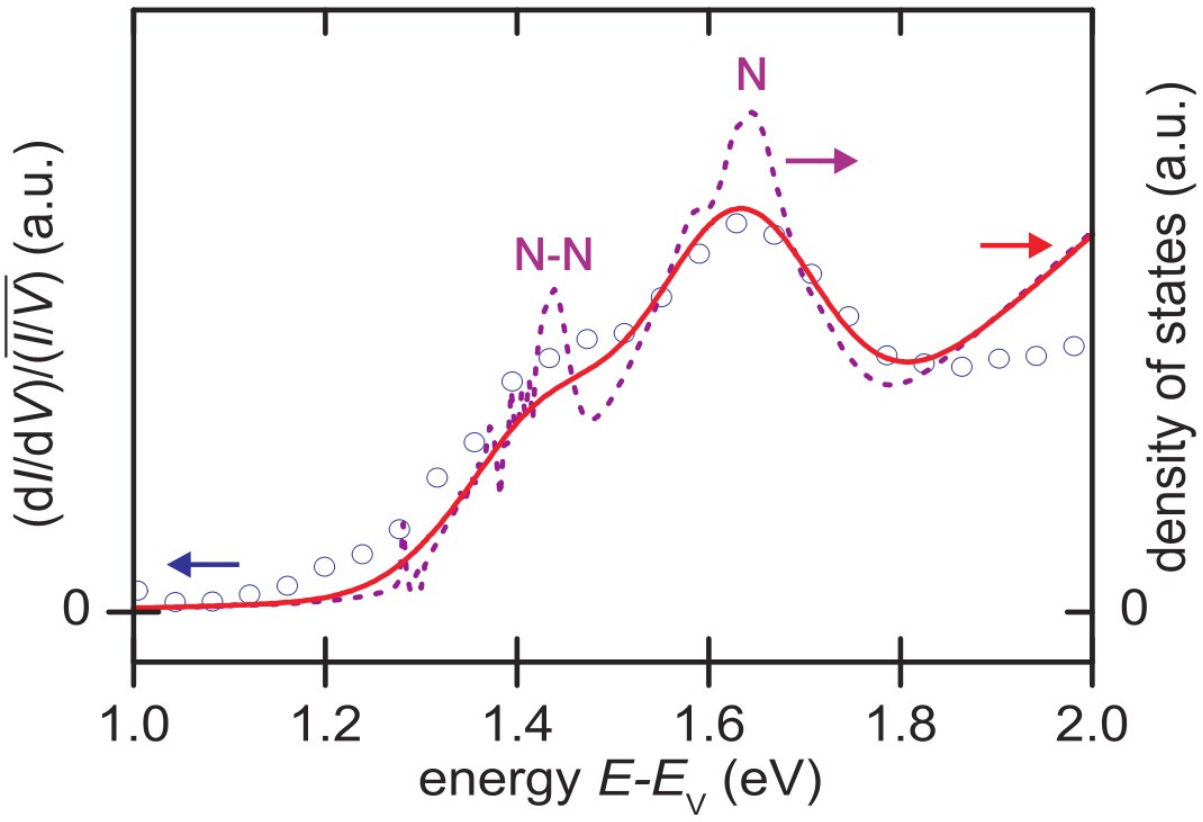


Circles:
Normalised differential conductivity measured for a GaNAs sample with x = 1.2%

Measured at T = 300 K

Red solid line:
Calculation of the density of states using LCINS data with thermal and modulation broadening folded in.

N.B: After identifying the band edges, the only fitting parameter used here is the overall scaling.



Circles:
STS data points

Dashed line:
Calculated DOS **without** extrinsic broadening effects folded in.

Solid line:
Calculated DOS with thermal and modulation broadening folded in.

Note that we can clearly identify features in the measured DOS associated with isolated N states and N-N pairs.

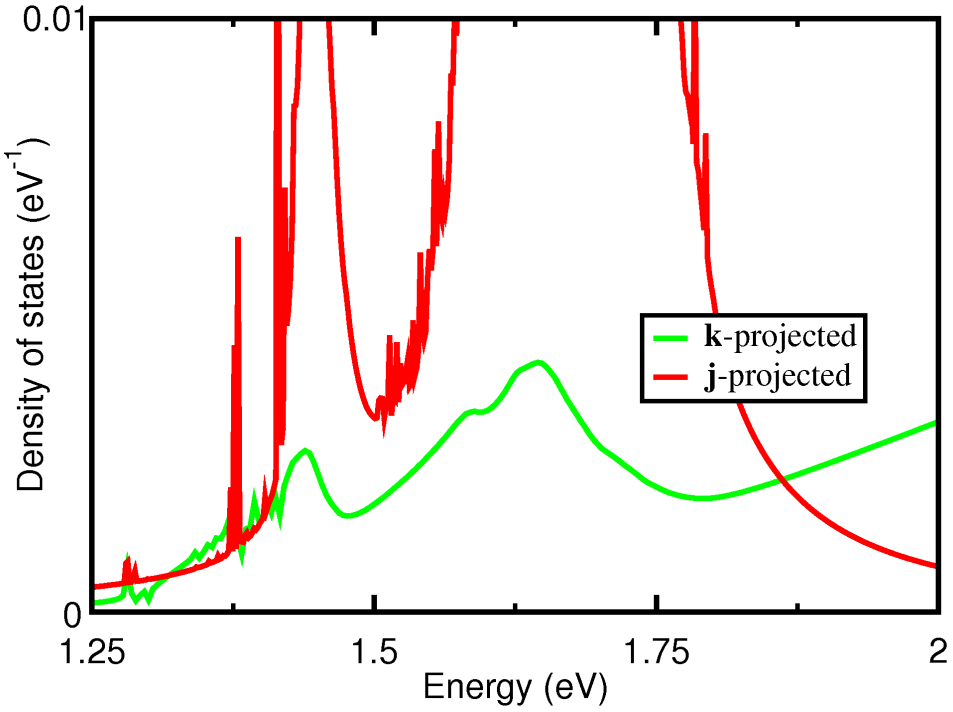
Absence of DOS projected onto N-states

The total density of states should also include the projection on to the N-states

$$D(E) = -\frac{1}{\pi}\mathrm{Im}\left(\sum_{\mathbf{k}} G(E, E_{\mathbf{k}}) + \sum_{\mathbf{j}} G(E, E_{\mathbf{j}})\right)$$

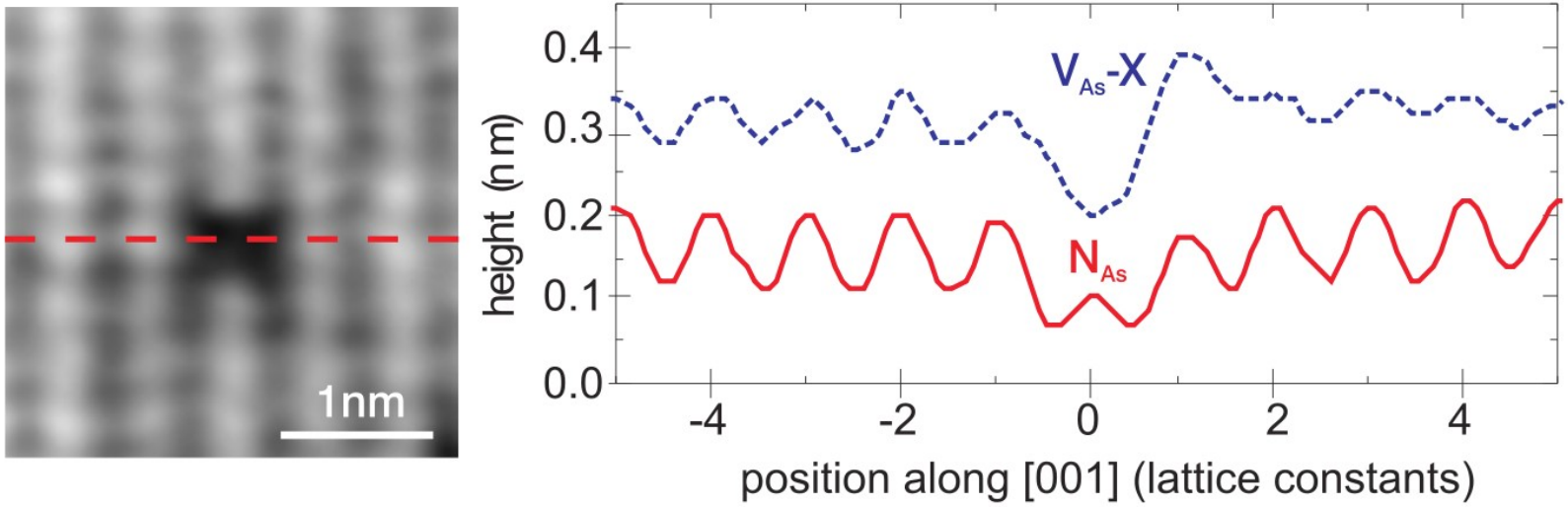
The second term is extremely large in comparison with the first, as shown left.

Why is this dominating term not present in the STS data?



STS samples the local density of states. At the surface, an N atom may relax away from its bulk tetrahedral formation, eliminating the resonant state in a similar fashion to hydrogen passivation.

Evidence for this is seen in the XSTM measurements shown below.



XSTM image of GaNAs surface showing N-site (left). The height profile taken along the dashed line is shown on the right. Note presence of dangling bond at N-site consistent with inward relaxation of the other three bonds.

Conclusions

- STS measurements have directly probed the local density of states in GaNAs
- These data have been successfully modelled using LCINS data within a Green's function formulation without arbitrary fitting parameters
- On the basis of this modelling, we may identify features in the STS data associated with isolated N states and N-N pairs
- The fine structure of the DOS is broadened by thermal and modulation broadening during the measurement process, suggesting that this structure may be explored in more detail by eliminating these effects as much as possible
- The absence of a contribution to the STS data from the DOS projected on to the impurity states may be explained in terms of surface relaxation of the N atoms
- Evidence for this explanation has been observed in XSTM data

Acknowledgements

LCINS state and interaction energies calculated by

Dr Andrew Lindsay

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