

Effect of Heavy Doping on Conduction Band Density of States: Implications for Device Modelling

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Abstract

In this paper, the doping induced distortion to the conduction band density of states is calculated by considering the many-body interactions of the electron-impurity system, following the work of Schwabe *et al.*, [3]. The results demonstrate that, at a high impurity density, the majority of states within the band tail are extended in real space and therefore contribute to current flow. Thus, a hydrogenic donor description is inappropriate for devices such as HBTs and HEMTs. For doping densities typically occurring in MESFETs, however, there is still a significant portion of donor states which are localised. The assumption of complete ionisation of donors may, therefore, lead to errors when modelling MESFETs.

I Introduction

In recent years, the inclusion of heavily doped layers within heterostructure based devices has become more widespread. It is common for pseudomorphic HEMTs to incorporate a very narrow and heavily doped donor layer, often described as δ or planar doping, in order to supply electrons to the conducting channel. Typically a few monolayers are grown epitaxially with a sheet donor density of $5 \times 10^{12} \text{ cm}^{-2}$ which translates to a density of $1 \times 10^{20} \text{ cm}^{-3}$. It is common to assume complete ionization of donors in the case of MESFETs. Some authors have introduced a hydrogenic-like shallow donor level when considering parasitic charge build up in HEMTs. In this work, the distortion to the density of states (DOS) is accounted for via a multiple scattering approach described in [1] in order to consider the density of localised states for various donor concentrations.

II Theory

The interacting electron-impurity system can be described using the one-electron Green's function,

$$G(\mathbf{k}, E) = \frac{1}{E - \epsilon(\mathbf{k}) - \Sigma(\mathbf{k}, E)} \quad (1)$$

where E and \mathbf{k} are the electron energy and wave-vector respectively. The function, $\epsilon(\mathbf{k})$, defines the eigenvalues of the unperturbed system,

$$\epsilon(\mathbf{k}) = \hbar^2 k^2 / 2m^* \quad (2)$$

Many-particle interactions are accounted for via the self-energy, Σ ,

$$\Sigma(\mathbf{k}, E) = \Sigma_{xc}(\mathbf{k}, E) + \Sigma_{e-i}(\mathbf{k}, E) \quad (3)$$

where Σ_{ec} and Σ_{e-i} refer to electron-electron and electron-impurity interactions respectively.

The DOS is then derived from the spectral density,

$$A(\mathbf{k}, E) = \mp \frac{1}{\pi} \Im \{G(\mathbf{k}, E \pm i0)\} \quad (4)$$

$$\rho(E) = \frac{1}{\Omega} \sum_{\mathbf{k}, \sigma} A(\mathbf{k}, E) \quad (5)$$

The self-energy is calculated using Klauder's 5th multiple scattering approximation, [2],

$$\Sigma_{e-i}(\mathbf{k}, E) \equiv U(\mathbf{k}, \mathbf{k}, E) - N_D V(0) \quad (6)$$

$$U(\mathbf{k}, \mathbf{q}, E) = N_D V(\mathbf{k} - \mathbf{q}) + \frac{1}{(2\pi)^3} \int d^3 q' V(\mathbf{q}' - \mathbf{q}) G(\mathbf{q}', E) U(\mathbf{k}, \mathbf{q}', E) \quad (7)$$

Schwabe *et al* [3] point out that the exchange-correlation contribution to the self-energy results in a rigid shift to the band edge and so has been omitted from the calculation.

The impurity potential, which includes screening via the inverse screening length, κ , is given by,

$$V(\mathbf{q}) = -\frac{4\pi e^2}{\epsilon_s} \frac{1}{q^2 + \kappa^2} \quad (8)$$

The Separable Potential Approximation transforms the integral equation into a secular equation, the roots of which define the DOS at a particular E.

$$V(\mathbf{q} - \mathbf{q}') = ZC(d)V^{1/2}(q)V^{1/2}(q') \quad (9)$$

$$\Sigma(\mathbf{k}, E) = -\frac{4\pi}{k^2 + \kappa^2} N_D S(E) \quad (10)$$

$$\begin{aligned} & \left[\frac{1}{2}(\kappa^2 - E) - \left\{ \frac{(\kappa^2 + E)^2}{4} + 4\pi N_D S(E) \right\}^{1/2} \right]^{1/2} + \\ & \left[\frac{1}{2}(\kappa^2 - E) + \left\{ \frac{(\kappa^2 + E)^2}{4} + 4\pi N_D S(E) \right\}^{1/2} \right]^{1/2} + \\ & Z - \frac{1}{S(E)} = 0 \end{aligned} \quad (11)$$

$$\rho(E) = \frac{1}{4\pi^2} \Im \left\{ \frac{1}{S(E)} - Z - (\kappa^2 + E) \frac{S(E)}{1 - ZS(E)} \right\} \quad (12)$$

III Results and Discussion

Figure 1 shows the density of states for various donor concentrations. At low donor densities an impurity band is formed which slowly merges with the conduction band density of states, usually described by $CE^{1/2}$, until a band tail is formed. It is clear from the figure that the transfer from impurity band to band tail occurs at a low doping density of around 5×10^{15} donors cm^{-3} .

In order to investigate the spatial behaviour of the electron wavefunction, the spectral density has been considered in figure 2, defining the probability that an electron with energy E is in state k . The doping density has been used at which the transition from impurity band to band tail takes place. The transition from localised to free states can clearly be seen where the spectral density changes from a function distributed in k -space with a maximum at $k = 0$ to a function which exhibits a well defined maximum at some finite value of k . This follows from the uncertainty principle with a small value of Δk implying a state that is extended in real space. The degree of localisation can be estimated using $R = A(k = 0)/A_{max}$, [1].

GaAs

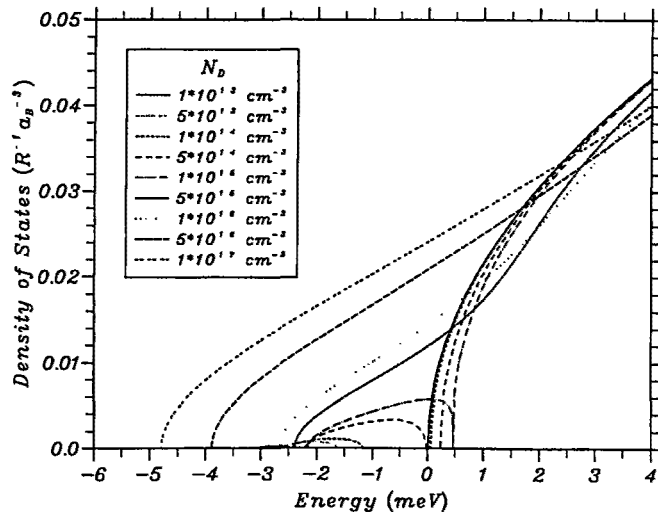


Figure 1: Effect of donor concentration on conduction band density of states.

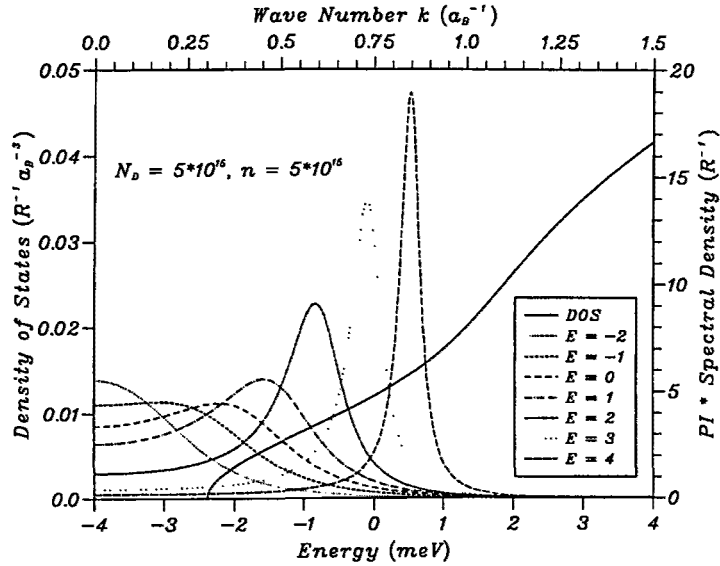


Figure 2: Spectral density distributions from localised to free states.

Figure 3 shows the ratio of localised state density to donor density as a function of impurity density. The localised state density is calculated by integrating the density of states function from the band tail edge to the point at which the transfer from localised to free states takes place. Serre and Ghazali define this transition at $R = 10\%$. As the impurity density is reduced in the low concentration regime, the localised state density approaches the donor density as predicted by the hydrogenic donor description. At higher doping densities, however, it is clear that the hydrogenic description is inappropriate with there being less than 10% of donor states which are localised (N_D greater than $1 \times 10^{18} \text{ cm}^{-3}$). Interestingly, at doping levels typically occurring in MESFETs (10^{17} donors cm^{-3}) there is still between 10 % and 30 % of donor states which are localised. At high doping densities, greater than 1×10^{19} , the majority of states are extended in real space and therefore contribute to a conduction band current.

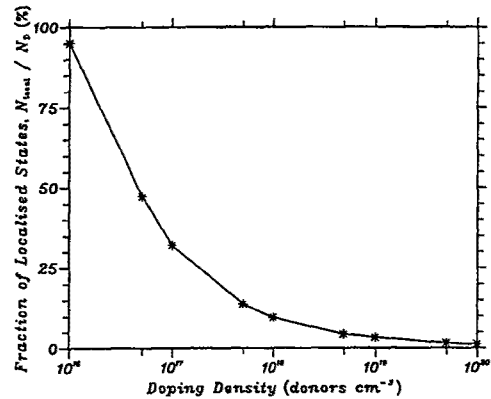


Figure 3: Fraction of localised donor states as a function of impurity concentration.

IV Conclusion

The analysis has shown that the hydrogenic donor model is invalid for doping concentrations typically occurring in HBTs, MESFETs, and HEMTs. Furthermore, the assumption that all donors are ionised appears to be incorrect for doping densities typically occurring in MESFETs. This approximation does, however, seem appropriate for HBTs and HEMTs where the doping density is typically greater than $5 \times 10^{18} \text{ cm}^{-3}$.

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References

- [1] J. Serre and A. Ghazali. From band tailing to impurity-band formation and discussion of localization in doped semiconductors: A multiple-scattering approach. *Phys. Rev. B*, 28(8):4704–4715, 1983.
- [2] J.R. Klauder. The modification of electron energy levels by impurity atoms. *Annals of Physics*, 14:43–76, 1961.
- [3] R. Schwabe, A. Haufe, V. Gottschalch, and K. Unger. Photoluminescence of heavily doped n-InP. *Solid State Communications*, 58(7):485–491, 1986.