

International Workshop on Computational Nanotechnology

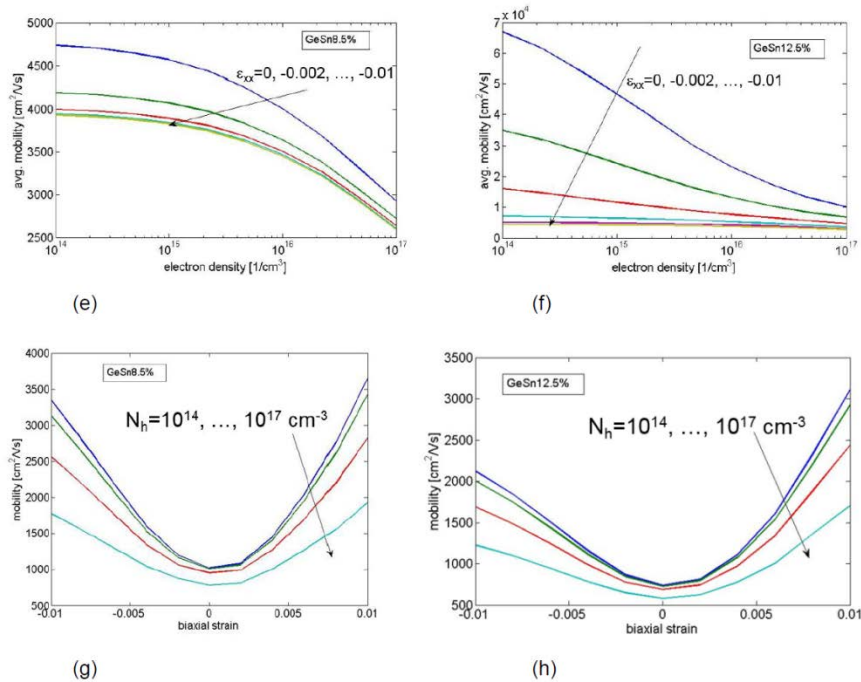


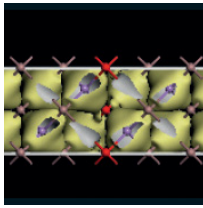
Fig. 1. (a,c) GeSn c.b. valley edges (solid) and Γ -population (dashed), low-density electron mobility (b,d), its dependence on electron density (e,f), and hole mobility (g,h) in strained GeSn at $T=300\text{K}$.

P:20 Transport modelling and design of GaN/AlN based unipolar (opto-)electronic devices, and interface quality effects

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The AlGaN/GaN material system has been proposed as a highly promising alternative to more conventional III-V's for various optoelectronic devices, e.g. quantum cascade lasers (QCL), photodetectors and electronic devices like resonant tunnelling diodes (RTD). The high LO-phonon energy in GaN should significantly reduce the thermal degradation effects coming from phonon-assisted relaxation, which could allow lasing at higher THz frequencies, and higher operation temperature [1]. A detailed understanding of electron transport in AlGaN/GaN heterostructures is crucial for optimizing devices performance. RTDs are interesting in their own right, and also as the simplest devices in which vertical tunneling and scattering transport can be investigated, both experimentally and theoretically: the experience can then be transferred to the design of more complicated devices. We have therefore investigated electron transport in epitaxially grown nitride-based RTDs, as well as in sequential tunneling devices [2]. The density-matrix model developed for this purpose is shown to be able to reproduce the experimental I-V characteristics. Scattering-induced broadening effects (largely coming from interface roughness) are found to have a strong influence on current magnitude and peak-to-valley ratios, highlighting critical optimization parameters for III-nitride unipolar electronic and optoelectronic devices. Investigation of AlGaN QCLs, also performed by the density matrix method, shows that a realistic level of interface roughness (found from RTD modelling) would degrade the



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gain and operating temperature of some previous designs. These can be improved by a structure optimization, based on a genetic algorithm [3], however further improvements of the material quality are essential for III-nitride QCLs to demonstrate their full potential.

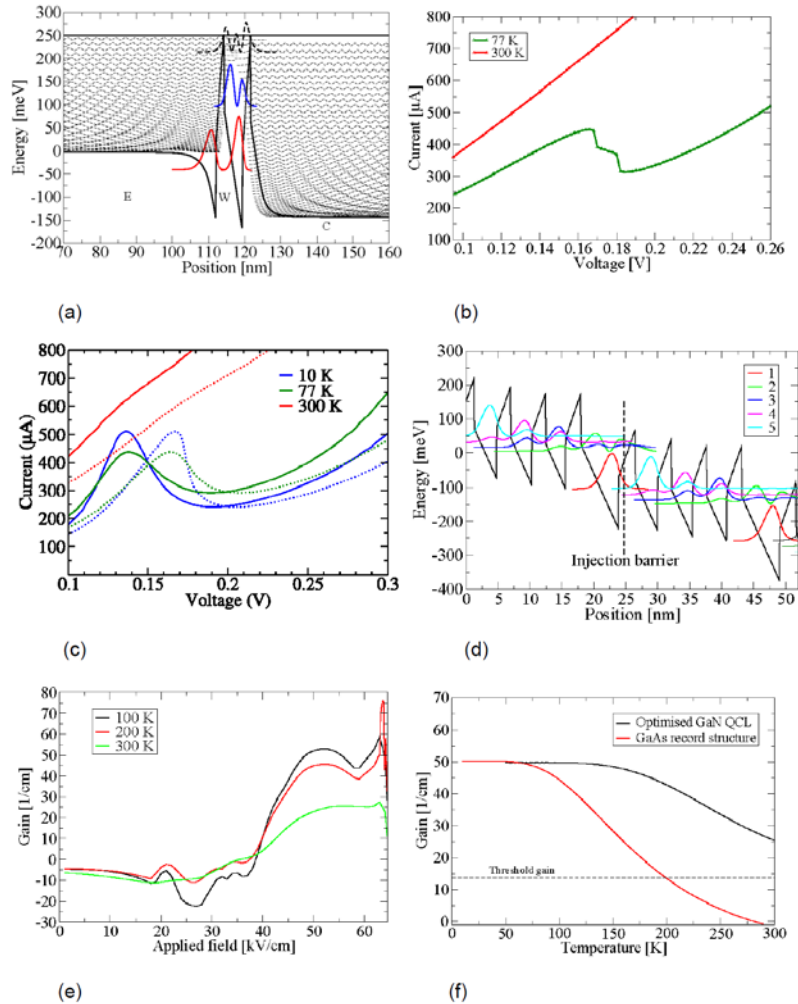


Fig.1. (a) $\text{Al}_{0.18}\text{Ga}_{0.82}\text{N}(4.9\text{nm})/\text{GaN}(2.4\text{nm})$ RTD structure and states, (b) measured and (c) calculated I-V characteristics for the interface roughness parameters $\Lambda=10\text{nm}$ and $\Delta=0.28\text{nm}$, (d) optimised $2.6/3.5/2.2/3.3/2.2/3.1/2.4/5.9\text{nm}$ ($\text{Al}_{0.08}\text{Ga}_{0.92}/\text{GaN}$) QCL structure, its calculated (e) gain-bias, and (f) gain-temperature dependence.

- [1] E. Bellotti, K. Driscoll, T. D. Moustakas, and R. Paiella, "Monte Carlo study of GaN versus GaAs terahertz quantum cascade structures," *Appl. Phys. Lett.*, 92, 101112 (2008).
- [2] A. Grier, A. Valavanis, C. Edmunds, J. Shao, J. D. Cooper, G. Gardner, M. J. Manfra, O. Malis, D. Indjin, Z. Ikonić, and P. Harrison, "Coherent vertical electron transport and interface roughness effects in AlGaIn/GaN intersubband devices", *J. Appl. Phys*, 118, 224308 (2015).
- [3] A. Grier, "Modelling the optical and electronic transport properties of AlGaAs and AlGaIn intersubband devices and optimisation of quantum cascade laser active regions", PhD Thesis, University of Leeds, 2015.