The effects of inter-diffusion in Si–SiGe quantum cascade devices

Leon Lever*, Robert Kelsall*, Zoran Ikonic*, Ian Ross†, Jing Zhang‡, Mhairi Gass§, Paul Townsend¶, Douglas Paul¶, N Q Vinh‖ and Carl Pidgeon‖
*School of Electrical and Electronic Engineering
Woodhouse Lane, Leeds, LS2 9JT, UK.
†Department of Engineering Materials, Sir Robert Hadfield Building,
Mappin Street, Sheffield, S1 3JD, UK.
‡EXSS, Blackett Laboratory, Imperial College London,
Prince Consort Road, London, SW7 2BW, UK.
§SuperSTEM, Daresbury Laboratory, Keckwick Lane,
Daresbury, WA4 4AD, UK.
¶Cavendish Laboratory, University of Cambridge,
Madingley Road, Cambridge, CB3 0HE, UK.
‖School of EPS, Physics Department, David Brewster Building,
Heriot-Watt University, Edinburgh, EH14 4AS, UK.
Email: l.j.m.lever@leeds.ac.uk

There has been significant interest in the development of a silicon-based quantum cascade laser (QCL). As yet such lasers have only been realised in III–V materials but a Si/SiGe laser would provide a route to more cost effective devices due to the mature process technology [1]. The weaker temperature dependence of the inter-subband lifetimes resulting from the lack of polar optical phonon scattering [2] may also allow higher temperature operation than III-V QCLs.

Aberration corrected annular dark field (ADF) imaging and electron energy loss spectroscopy has been used to gain information about the Ge fraction profile at Si–SiGe interfaces in epitaxially grown hetrostructures for QCL applications. Fig. 1 shows an ADF image of a two quantum well Si–$Si_{0.6}Ge_{0.4}$ structure. The image contrast is proportional to the average atomic number (Z-contrast) hence Si barrier regions appear dark while SiGe quantum wells appear bright. The nominal dimensions for the narrow Si barrier is 8 Å with two 44 and 33 Å SiGe quantum wells respectively. The insert in Fig. 1 shows a Ge concentration profile across the region indicated in the ADF image. It is clear from the ADF image and Ge concentration profile that the interfaces are not abrupt and that the 8 Å Si barrier does not reach the nominal pure Si composition.

Measurements of the transition energy using the Dutch Free Electron Laser for Infrared eXperiments (FELIX) between heavy-hole ground states of the adjacent wells, as described for the structures in [3], show the transition to be 15 ± 1 meV. Using a 6×6 **k.p** model to calculate wavefunctions, and with an abrupt interface between nominal Ge fraction layers, a difference in energy of 10 meV is calculated between the two couple heavy-hole ground states. Using the same **k.p** model, but considering the Ge fraction as an error-function variation across the interface, and a diffusion length of 10 Å, the energy difference is 15.4 meV. Fig. 2 shows the simulated conduction band edge and probability density for the heavy-hole ground states.

Inclusion of the Ge inter-diffusion for bandstructure calculations in thin layer quantum confined heterostructures makes a significant difference to the calculated wavefunctions. The calculated bandstructures yield energies for subband states that are substantially closer to experimental observations.

Thin (<1 nm) barriers are expected to be an essential feature of any successful Si/SiGe quantum cascade laser. We have included the experimental inter-diffusion data in simulations of Si/SiGe laser structures, and will show the impact of interdiffusion on the electronic and optical properties of typical designs.

REFERENCES

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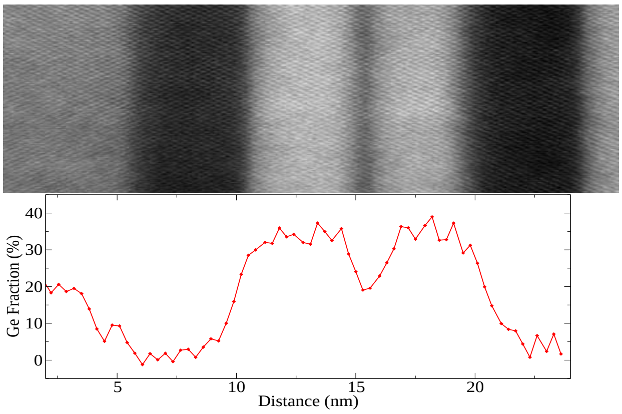

Fig. 1. Top: Aberration corrected ADF-STEM image along the growth direction (left to right) of Si–$Si_{1-x}Ge_x$ heterostructure, x=0.4. Image contrast is proportional to the average atomic number (Z-contrast) hence Si regions appear dark while $Si_{1-x}Ge_x$regions appear brighter. Bottom: Ge concentration profile.

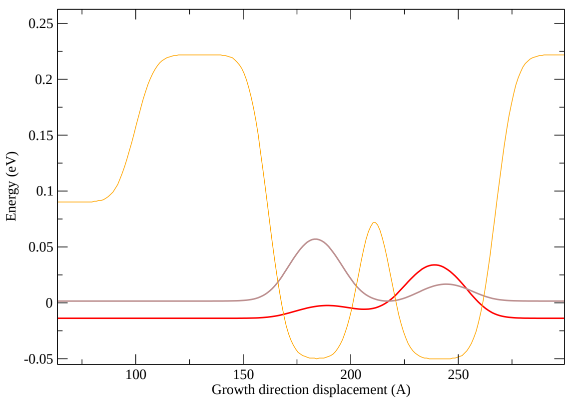

Fig. 2. Heavy-hole ground state wavefunctions with measured layer thicknesses and a diffusion length of 10 Å. The transition energy is 15.4 meV. Note that the energy scale is reversed, so that the ground state is lowest in energy.