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High-quality n-type Ge/SiGe multilayers for THz quantum cascade lasers

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.*Abstract* — **The exploitation of intersubband transitions in Ge/SiGe quantum cascade devices could pave the way towards the integration of THz light emitters into the silicon-based technology. Aiming at the realization of a Ge/SiGe Quantum Cascade Laser (QCL), we investigate optical and structural properties of n-type Ge/SiGe coupled quantum well systems. The samples have been investigated by means of X-ray diffraction, scanning transmission electron microscopy, atom probe tomography and Fourier Transform Infrared absorption spectroscopy to assess the growth capability with respect to QCL design requirements, carefully identified by means of modelling based on the non-equilibrium Green function formalism.**

I. INTRODUCTION

In the past 15 years, THz QCLs have been intensively developed using III-V materials, but the maximum temperature operation reported remains limited to 200 K due to the effective electron–polar phonon interaction [1]. In polar lattices, the longitudinal optical (LO) phonons induce a long-range polarization field which strongly couples to the charge carriers through the Fröhlich interaction. The THz transitions are typically designed to be well below the LO phonon energy (36 meV), so that at low temperature the upper laser state is protected against relaxation by emission of LO-phonons. Increasing the temperature, however, the thermally activated electrons in the subband of the upper lasing state gain enough in-plane kinetic energy to access this scattering channel. This non-radiative relaxation of carriers reduces the population inversion and is responsible for quenching of the laser emission with increasing temperature as the gain drops below the cavity losses. From this perspective, implementing the THz QCL architecture on non-polar SiGe multilayers has great technological relevance. Indeed in these crystals the electron–phonon coupling is controlled by the deformation potential which due to its short range is much less effective than the Fröhlich interaction. Thus, the maximum gain for a Ge/SiGe QCL is expected to be more robust against the temperature increase with respect to III-V based devices.

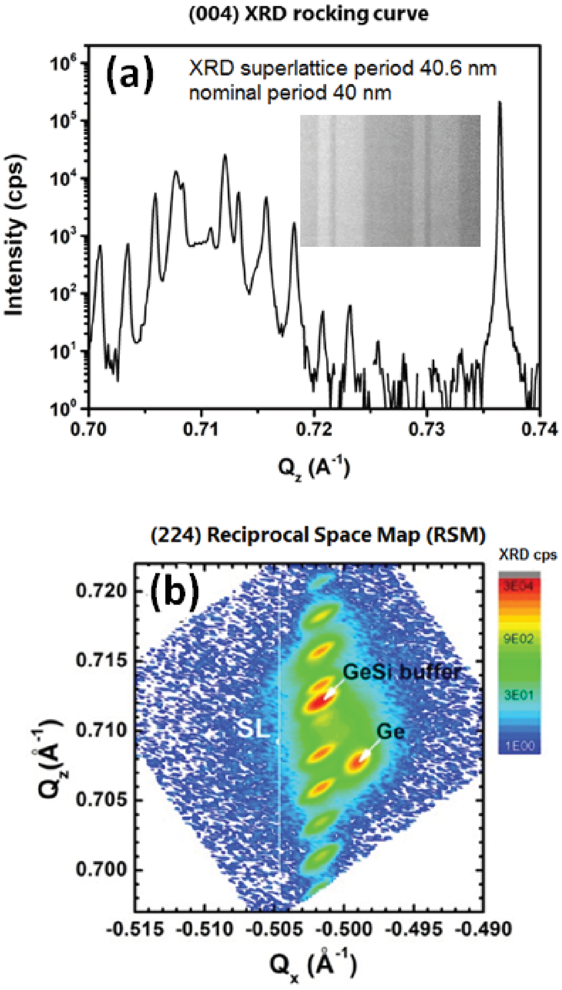

Fig. 1. XRD rocking curve around the 004 reflection (a) and reciprocal space maps around the (224) reflections (b) of a Ge/SiGe ACQW sample. In the inset of (a) the STEM image shows 2 periods of the structure.

The first THz electroluminescene in the SiGe/Si system came from p-type designs [2] but the high effective mass and strong mixing of subband states from non-parabolicity significantly limits the gain [3]. Amongst different configurations (electron or hole based, Si or Ge rich regimes), theoretical and experimental studies have indicated that n-type Ge/SiGe heterostructures, where the charge transport is associated to L-valley electrons, as the most promising architecture [1-8]. Progress in chemical vapour deposition (CVD) epitaxial growth makes now possible the deposition of high-quality n-type strain compensated Ge/SiGe multilayers on Si substrates leveraging on the reverse graded high Ge content SiGe virtual substrate

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approach. Sharp intersubband (ISB) THz absorption peaks in the 20–50 meV region with an upper energy state characterized by long and temperature-robust non-radiative lifetime have been measured [4-6]. Here we investigate n-type Ge/SiGe coupled quantum well systems with atomic level structural studies in order to assess the growth capability with respect to QCL design and performance requirements.

II. RESULTS

A 20 period stack of n-type strain-symmetrized Ge/$Si_{0.2}Ge_{0.8}$ asymmetric coupled quantum wells (ACQW) consisting in wide and narrow Ge quantum wells separated by a tunneling barrier with thicknesses w_L, w_t, b_t, respectively, have been grown at 500 °C on Si(001) substrates by ultrahigh vacuum CVD. The wide well has been codoped by phosphine resulting in a sheet electron density n_{2D} of approximately 7×10^{11} cm^{-2}.

X-ray diffraction measurements are shown in Fig. 1 and demonstrate the high quality of the material with good control of the compositional and geometrical profiles along the entire strain symmetrized active stack. Scanning transmission electron microscopy (STEM) provides evidence for the presence of sharp heterointerfaces (see the inset in Fig. 1 (a)).

We have studied the coupling between the electron states in adjacent quantum wells by means of Fourier Transform Infra-Red (FTIR) absorption experiments to probe the intersubband transitions. The measured 2D absorbances of the ACQWs having well widths w_L=12 and w_t=5 nm with different tunnel barrier thicknesses are shown in Fig. 2 (a). In Figs. 2 (b) and 2 (c) we report the square modulus of the electron wave funtions, calculated using a multivalley, self-consistent, Poisson-Schrödinger solver for b_t=8 nm (in the non interacting QW limit) and b_t= 2.3 nm (with strongly interacting QWs). In the latter case a reduced tunneling barrier height has been used in order to take into account the effect of intermixing, appreciable in the thinner barriers of the structure [7]. The decreasing of the tunneling barrier width results in an increase of the coupling between the two excited electron states. In agreement with these simulations we found that for barrier thickness narrower than 5 nm, two intersubband transition peaks are present in the absorption spectra whose energy separation increases by decreasing b_t. Our data unambiguously demonstrates control over the inter-well coupling and the electron tunnelling. These results combined with the modelling of non-radiative lifetimes, measured by pump-probe experiments, allowed us to design more complex structures in order to evaluate the key parameters driving electron scattering in this material system.

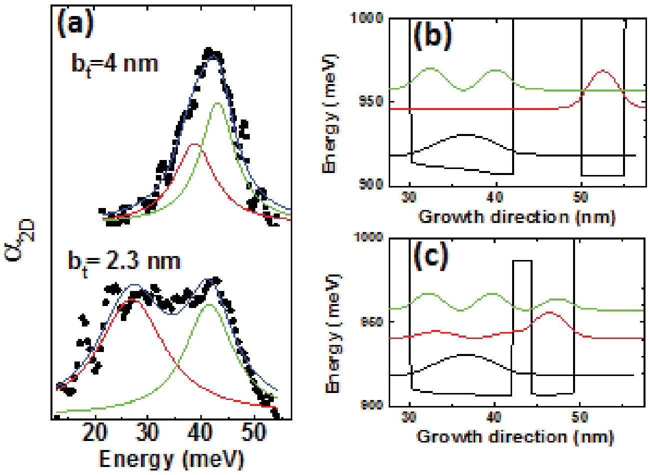

Fig. 2. (a) FTIR absorption spectra of the ACQW samples having well widths w_L=12 and w_t=5 nm and different tunneling barriers thickness b_t. (b), (c) square modulus of the electron wave functions of the ground and the first two excited states calculated in the limit of non-interacting quantum wll (b_t.=8nm) and for strongly interacting quantum wells (b_t.=2.3 nm).

Furthermore, to assess the potential of the Ge/SiGe material system as a gain medium for intersubband cascade devices, we used the non-equilibrium Green's function formalism to benchmark the performances of a Ge/SiGe 4-quantum well QCL against its GaAs/AlGaAs counterpart [8]. At low lattice temperatures, the Ge/SiGe QCL features a smaller gain with respect to the GaAs/AlGaAs device. This is attributed to its larger confinement effective mass and to a higher effective electron temperature, which results from a less efficient energy transfer from the carriers to the lattice. The material gain, however, turns out to be much more temperature insensitive. In fact, while in the GaAs/AlGaAs system the laser amplification rapidly quenches above 150 K, in the Ge/SiGe case a positive optical gain of 20 cm^{-1} is predicted at room temperature. Although interface roughness has a large detrimental impact on the gain we found that the small interface height of our samples, measured by means of atom probe tomography, can allow laser operation up to room temperature in optimized structures featuring low waveguide losses.

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