Conceptual design improvements for terahertz quantum cascade lasers needed for molecule detection

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Summary: Security and gas sensing applications such as the nonintrusive detection of concealed weapons and the rapid detection of chemicals and explosives require a failsafe identification of complex molecules. Since many excitation lines of complex molecules lie in the terahertz (THz) regime of the light spectrum, these applications require coherent and intense THz light [1]. Promising candidates for efficient and coherent THz light emission are THz quantum cascade lasers (THz-QCLs). So far, the operation of these lasers is limited to cryogenic temperatures. Recent theoretical and experimental work, however, have shown significant performance improvements. This suggests that operating THz-QCLs at temperatures beyond the limit of active cooling devices is feasible with a proper, still to be found THz-QCL design. Disadvantages in the design of state of the art THz-QCL are analyzed and alternative design concepts are combined within a concrete THz-QCL proposal. The design improvements are 1) suppression of electronic heating, 2) indirect pumping of the upper laser levels, 3) nonlocal optical transitions, 4) usage of materials with low effective electron masses and 5) a concrete growth orientation to protect the laser performance from growth variations. Nonequilibrium Green's function calculations of the stationary current and the optical gain of the proposed THz-QCL show a higher optical gain, an increased maximum laser operation temperature and a lower threshold current density compared to the conventional design.

In this work, several conceptual THz-QCL device improvements are presented, theoretically evaluated and combined into a concrete THz-QCL proposal: 1) The energy balance between electron transport and phonon emission is revised to reduce electronic heating effects to a minimum. 2) Upper laser levels are pumped via resonant phonon emission instead of coherent electron tunneling to achieve highest occupation inversions. 3) The optical transitions are designed to be nonlocal to suppress nonradiative losses. 4) Materials of low effective electron masses are combined to enhance the optical transition matrix elements. 5) It is suggested to orient the rougher interfaces of quantum barriers towards the drain to stabilize the laser performance against growth quality issues.

The electronic transport and the optical gain of all QCLs in this work are calculated using the nonequilibrium Green's function method including incoherent scattering on phonons, impurities, rough interfaces and alloy disorder in the self-consistent Born approximation. Electron-electron scattering is included in Hartree approximation. The QCLs are treated as open devices with periodic semi-infinite leads which mimic repeated supercells efficiently.

The proposed THz-QCL consists of $In_{.53}Ga_{.47}As/GaAs_{.51}Sb_{.49}$ layers [2]. Starting from the leftmost barrier in Fig. 1, one period of the QCL sequence was taken as **2.7**/<u>9</u>/**1.8**/20.7/**2.7**/15.3/**2.7**/18.9 nm. The bold and regular numbers represent $GaAs_{.51}Sb_{.49}$ and $In_{.53}Ga_{.47}As$ layers, respectively. The underlined 9-nm thick quantum well is the only n-doped region at the level of 2.04×10^{16} cm^{-3}. The contour plot in Fig. 1 shows the spectral function A(z,E) of the proposed QCL at zero in-plane momentum resulting from this NEGF calculation. Resonant states correspond with peaks of A(z,E) and illustrate several of the before mentioned features: 1) The total potential drop per period agrees with the energy of two longitudinal optical phonons (LO-phonons) to prevent heating of the electron gas. 2) The upper laser level #4 is filled with electrons from state #5 by resonant emission of LO-phonons. 3) The lower laser level #3 is spatially separated from state #4 to prevent nonradiative losses between the laser levels.

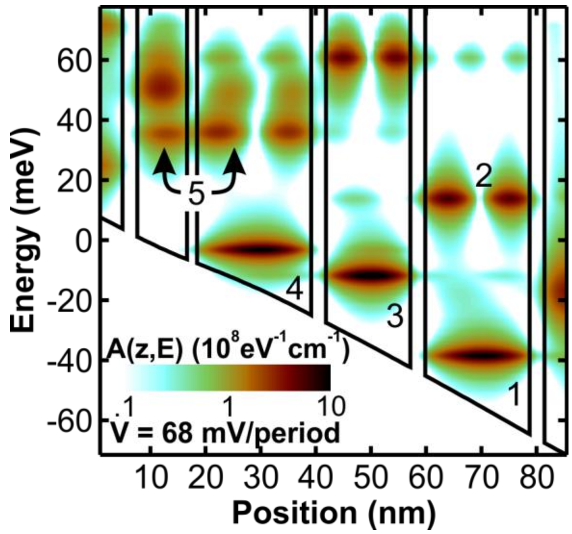

Figure 1. Calculated conduction band profile (line) and contour plot of the energy and spatially resolved spectral function A(z,E) at vanishing in-plane momentum in the proposed QCL at the threshold bias voltage of 68mV per period and a lattice temperature of 100K. The zero in energy marks the chemical potential of the source.

Figure 2 shows the calculated peak optical gain as a function of the QCL temperature for a conventional resonant phonon QCL of [3] and the proposed QCL of this work [2]. The combined improvements of the proposed QCL yield an about 10 times higher optical gain for all device temperatures. Accordingly, the maximum operation temperature is about 50K higher than in the conventional design. In addition, the threshold current density of the proposed design is about four times smaller than in the conventional design of the same effective doping and temperature.

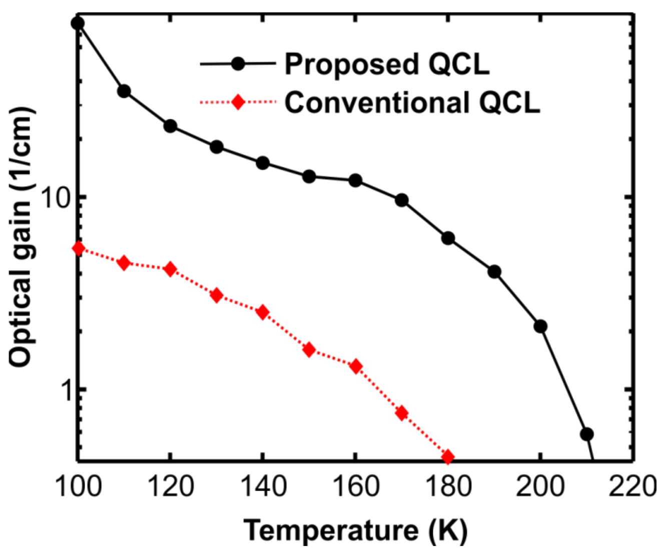

Figure 2. Optical gain as a function of device temperature in the conventional THz-QCL of [3] and of the proposed THz QCL design of [2].

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