Microscopic modeling of second harmonic generation in quantum cascade lasers

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During the last 20 years since the first Quantum Cascade Laser (QCL) [1] there has been substantial development. The long-wavelength limit exploiting intersubband transitions below the reststrahlenband with frequencies in the terahertz range [2] is currently an area of active research but efforts are also being made in the opposite direction towards the short-wavelength limit. As the lasing is based on intersubband transitions with relaxation and thus gain recovery times of picoseconds, they far exceed the solid state lasers when it comes to modulation speed [3]; although the frequencies are limited by the conduction band offset. Possible high speed applications makes it worthwhile to try to extend the wavelength regime towards the telecom frequencies.

In this work our implementation of the Keldysh non-equilibrium Green's function (NEGF) formalism [4] is applied to the phenomena of frequency doubling, i.e. second harmonic generation, which is a straightforward way to achieve shorter wavelengths. The key concept here is that the time dependence of each observable is expressed as a Fourier series with the driving frequency as the fundamental frequency, an approach originally proposed by Brandes [5]. As an example, average current is expressed in this form as

$$J(t) = J_0 + \sum_n J_n^{\cos} \cos(n\omega_0 t) + J_n^{\sin} \sin(n\omega_0 t). \tag{1}$$

The second order terms J_2 will be the signature of second harmonic generation. The truncation of this Fourier space in n gives us the possibility of stepwise introducing higher orders of response, basically giving another set of convergence criteria in the simulations.

The laser field is considered as a classical field oscillating at frequency ω_0 and with this formalism it can be included with finite field strength in comparison to linear response implementations. In addition to the finite field strength, the full quantum mechanical description is provided by the self-consistently calculated self-energies containing the most relevant scattering mechanisms.

The simulation results here are based on a structure labeled D2912 [6] which was designed to improve the conversion efficiency. In short, the idea was to integrate the pump and the nonlinear element in the same active region of the heterostructure and thus avoid the saturation of the pump intensity.

The model used provides reasonable agreement for the current through the structure (Fig. 1) and gain simulations show that there should be a clear increase in intensity with current (Fig. 2 and 3). A particular effect that can be observed at high intensity is a dip in conversion efficiency in the middle of the window of operating biases as shown in Fig. 4. The dip is indeed seen in the experiment [6], where it was attributed to the activation of higher modes in the waveguide. Our results provide an alternative explanation based on a full microscopic modelling of the operating laser.

REFERENCES

[1] J. Faist, F. Capasso, D.L. Sivco, C. Sirtori, A.L. Hutchinson, A.Y. Cho, Science **264**, 553 (1994)
[2] B.S. Williams, Nature Phot. **1**, 517 (2007)
[3] Y.H. Cho, A. Belyanin, Journal of Applied Physics **107**(5), 053116 (2010)
[4] A. Wacker, M. Lindskog, D. Winge, Selected Topics in Quantum Electronics, IEEE Journal of **99**, 1200611 (2013)
[5] T. Brandes, Phys. Rev. B **56**, 1213 (1997)
[6] C. Gmachl, A. Belyanin, D.L. Sivco, M.L. Peabody, N. Owschimikow, A.M. Sergent, F. Capasso, A.Y. Cho, Quantum Electron., IEEE Journal of **39**, 1345 (2003)

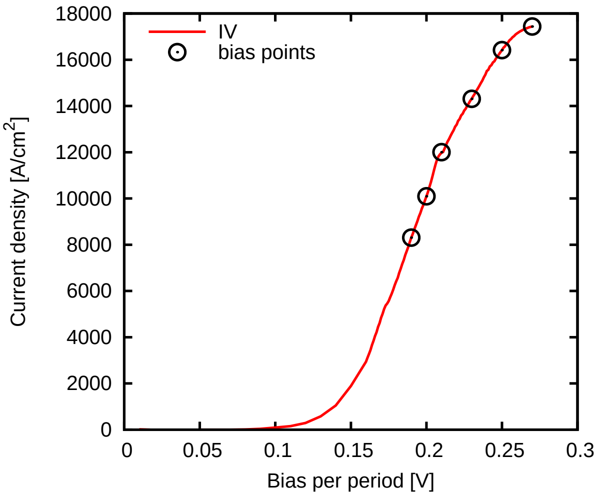

Fig. 1. Current versus voltage characteristics of structure D2912 [6]. Further simulations have been made at the marked bias points 190, 210, 230, 250 and 270 mV per period.

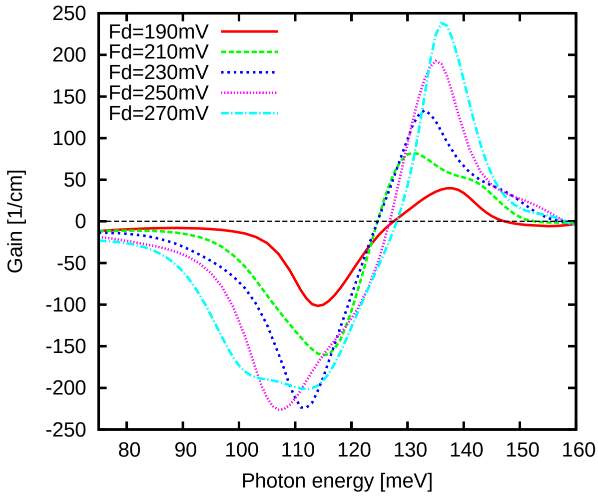

Fig. 2. Simulated gain at the bias points marked in Fig. 1. Sufficient gain to overcome the losses is reached already at 190 mV per period, which is consistent with experimental findings [6].

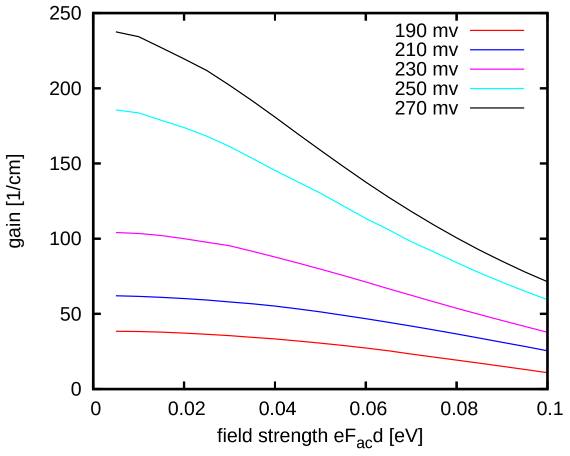

Fig. 3. Gain versus ac-field strength of the lasing field. One observes clear saturation with lasing intensity. Even though, the simulated data shows that the gain of the structure is capable of overcoming threshold gain (which should be less than 20 cm^{-1}) at high ac field strength.

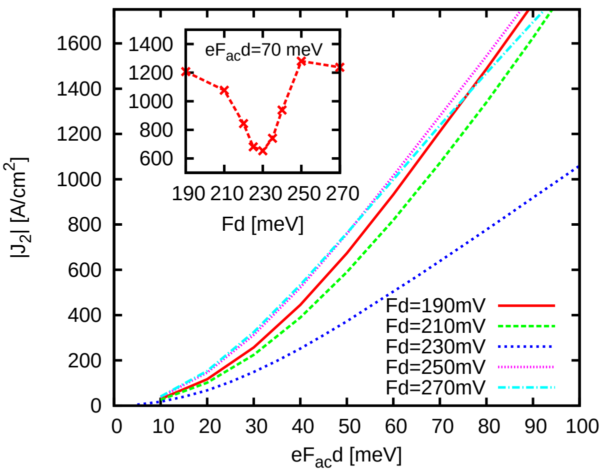

Fig. 4. Simulated second order current response. Conversion efficiency is nearly constant despite at biases around 230 mV. Inset: Second order current at constant field strength to emphasize the effect on the conversion efficiency.