Modeling and numerical simulation of electrically pumped single-photon emitters

Markus Kantner, Uwe Bandelow, Thomas Koprucki and Hans-Jürgen Wünsche

Weierstrass Institute for Applied Analysis and Stochastics
Mohrenstr. 39
10117 Berlin, Germany
Email: kantner@wias-berlin.de

***Abstract*—Semiconductor quantum dots are promising candidates for the realization of electrically pumped single-photon sources. The numerical simulation of such devices has to deal with cryogenic temperature effects and suitable models for the quantum dot occupation and single-photon generation. We demonstrate some first steps in a hybrid approach for the simulation of electrically pumped single-photon sources by coupling the semiconductor transport equations to a quantum mechanical model for the microscopic physics.**

I. Introduction

Single-photon emitters are opto-electronic devices that ideally emit a single photon in response to an external excitation. Such devices enable many interesting applications such as quantum key distribution, quantum repeaters, quantum metrology and quantum computing [1], [2]. A promising candidate for electrically driven single-photon sources are semiconductor quantum dot (QD) based devices. QDs provide an excellent representation of two-level systems and can be grown in semiconductor micro-cavities by well established fabrication techniques. Numerical simulation of carrier transport and single-photon generation can help to study the device performance and enhance its efficiency.

II. Device concept and charge carrier transport at cryogenic temperatures

On a macroscopic level the charge carrier transport can be studied in the framework of the van Roosbroeck system [3] which is a coupled system of the nonlinear Poisson's equation for the electrostatic potential ψ

$$-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla \psi = q\left(p - n + N_D^+ - N_A^-\right) \tag{1}$$

and a continuity equation for each carrier species

$$\begin{aligned} q\partial_t p + \nabla \cdot \mathbf{j}_p &= -qR\left[\psi, p, n\right], \\ q\partial_t n - \nabla \cdot \mathbf{j}_n &= -qR\left[\psi, p, n\right]. \end{aligned} \tag{2}$$

Here n denotes the electron density, p is the hole density, q is the elementary charge, ε_r is the dielectric constant of the semiconductor, ε_0 is the vacuum permittivity and R models various recombination mechanisms (Shockley-Read-Hall recombination, Auger recombination, radiative recombination). The current densities $\mathbf{j}_n$ and $\mathbf{j}_p$ are modeled in a standard way as drift and diffusion currents [4], [5]. The device layout considered here is a GaAs-based p-i-n structure with a non-planar surface on top. It has been shown that such non-planar structures can significantly enhance the photon extraction efficiency by reduction of the total internal reflection [6]. In the center of the intrinsic domain a very thin film of InGaAs is grown epitaxially on the GaAs substrate. The lattice mismatch induced strain in the material composition causes the self-organized formation (Stranski–Krastanov growth mode) of a wetting layer (WL) and quantum dots (QD).

The device is designed for operation at $T = 30\,\mathrm{K}$ to ensure the existence of bounded states in the InGaAs-QD and a small emission linewidth. In this situation the thermal energy is ten times smaller than at room temperature and therefore several aspects of device simulation become important that are insignificant at room temperature but crucial in the cryogenic limit.

The carrier densities are governed by the chemical potentials which scale with the thermal energy $k_B T$. Consequently small differences between the band edge energy and the carriers quasi Fermi potential are exponentially enhanced and result in domains with either a very low (depleted semiconductor) or very high (degenerated semiconductor) carrier densities, separated by extremely narrow boundary layers. In this case the carrier densities need to be described by the Fermi-Dirac distribution - the Boltzmann approximation is not valid anymore at cryogenic temperatures. Another important aspect is the incomplete ionization of the built-in dopants. At $30\,\mathrm{K}$ the carriers tend to freeze out if the built-in impurity concentration is below the critical impurity density for the Mott metal-insulator transition. The activated net doping in Eq. (1) can differ significantly from the built-in dopant concentrations and must be computed from

$$N_D^+ = \frac{N_D}{1 + 2e^{(E_{F_n} - E_D)/k_B T}}$$

and

$$N_A^- = \frac{N_A}{1 + 4e^{(E_A - E_{F_p})/k_B T}}$$

along with a suitable model for the activation energies E_A and E_D [5], [7]. Moreover, we consider models for the energy band

978-1-4799-8379-7/151$31.00 ©2015 IEEE

gap and carrier mobilities that take the impurity density and temperature dependence into account.

We study the carrier supply for the QD and the current flow in the device in the low and moderate injection regime. Transient numerical simulations indicate that the device follows electrical pulses on a very fast timescale such that the maximum operation frequency is set by the radiative lifetime of the excitons in the QD. The numerical simulations are performed using the software package WIAS-TeSCA [8] based on a finite volumes Scharfetter-Gummel method [9].

III. Quantum dot occupation and photon kinetics

The core element of the device is the QD, where the electron-hole-recombination and single-photon generation takes place. This section of the device is described in the framework of cavity quantum electrodynamics as an open quantum system coupled to the surrounding device as an external reservoir. For simplicity, we consider the QD as a two-level system which can be either empty or occupied by an exciton. The exciton-photon interaction is described by the Jaynes-Cummings Hamiltonian

$$H = \hbar\omega_0 a^\dagger a + \hbar\left(\omega_0 + \delta\right) b^\dagger b + \hbar g \left(b^\dagger a + b a^\dagger\right),$$

where a and $a^\dagger$ are the annihilation and creation operators for the photons with energy $\hbar\omega_0$ obeying the bosonic commutator relation $\left[a, a^\dagger\right] = 1$. The capturing and recombination of the excitons is modeled by the operators b and $b^\dagger$ with the anti-commutator relation $\left\{b, b^\dagger\right\} = 1$. The exciton energy can be weakly non-resonant to the photon energy with a small detuning δ. The light-matter coupling constant g is determined by the dipole transition moment, the mode volume and the photon wavelength. The interaction of the QD with the carrier reservoir is modeled by a density matrix approach with a non-unitary time-evolution given by the Kossakowski-Lindblad equation

$$\partial_t \rho = -\frac{i}{\hbar}\left[H, \rho\right] + \kappa\mathcal{L}(a)\rho + \gamma\mathcal{L}(b)\rho + p\mathcal{L}(b^\dagger)\rho \qquad (3)$$

where $\mathcal{L}(a)\rho = a\rho a^\dagger - \frac{1}{2}\left\{a^\dagger a, \rho\right\}$ denotes the Lindblad super-operator [10]. The dissipative interactions of the QD with the reservoir considered in this model are:

1) photon emission from the cavity with a rate κ
2) spontaneous emission with a rate γ (exciton decay)
3) pumping of excitons from the reservoir into the QD with a rate p

It was shown earlier that the probability of multi-photon events can be strongly suppressed by pulsed electrical injection [11]. Thus we assume stationary as well as time-dependent pumping rates. The pumping rate $p(t)$ represents the coupling parameter between the macroscopic transport described by Eqs. (1) & (2) and the microscopic model Eq. (3). In order to study the dynamics of the QD state and the photon number, the quantum master equation (3) is projected on a finite-dimensional subspace that can be truncated at large photon numbers. The resulting set of ODEs is studied numerically by standard methods.

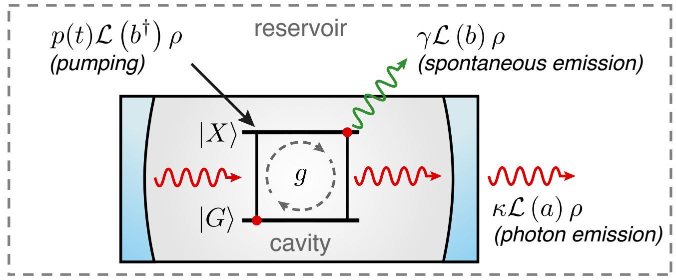

Figure 1. Dissipative interactions of the QD in a micro-cavity with an external reservoir and a quantized electromagnetic field. The microscopic physics is described by the quantum master equation (3).

IV. Summary

Numerical simulation of semiconductor-based single-photon sources requires the coupling of the drift-diffusion system to a microscopic model in order to display the carrier recombination and single-photon generation in the QD. In the case of arsenide-based material systems these devices need to operate at cryogenic temperatures which is a challenging task for numerical device simulation. In the framework of a quantum master equation we study the single-photon generation in a simple two-level system that is coupled to the device as an external reservoir.

Acknowledgment

This work has been supported by the Deutsche Forschungsgemeinschaft through SFB 787 “Semiconductor Nanophotonics” under grant B4.

References

[1] S. Buckley, K. Rivoire, and J. Vučković, “Engineered quantum dot single-photon sources,” *Reports on Progress in Physics*, vol. 75, no. 12, p. 126503, Nov 2012.
[2] V. Zwiller, T. Aichele, and O. Benson, “Quantum optics with single quantum dot devices,” *New Journal of Physics*, vol. 6, p. 96, Jan 2004.
[3] W. Van Roosbroeck, “Theory of the flow of electrons and holes in germanium and other semiconductors,” *Bell System Technical Journal*, vol. 29, no. 4, pp. 560–607, Oct 1950.
[4] P. A. Markovich, *The stationary Semiconductor device equations*. Wien: Springer, 1986.
[5] S. L. Chuang, *Physics of Photonic Devices*. Wiley, 2009.
[6] W. Barnes, G. Björk, J. Gérard, P. Jonsson, J. Wasey, P. Worthing, and V. Zwiller, “Solid-state single photon sources: light collection strategies,” *The European Physical Journal D - Atomic, Molecular and Optical Physics*, vol. 18, no. 2, pp. 197–210, Feb 2002.
[7] A. Akturk, J. Allnutt, Z. Dilli, N. Goldsman, and M. Peckerar, “Device modeling at cryogenic temperatures: Effects of incomplete ionization,” *IEEE Transactions on Electron Devices*, vol. 54, no. 11, pp. 2984–2990, Nov 2007.
[8] H. Gajewski, “Analysis und Numerik von Ladungstransport in Halbleitern,” *WIAS Report*, no. 6, 1993, ISSN 0942-9077.
[9] D. L. Scharfetter and H. K. Gummel, “Large-signal analysis of a silicon read diode oscillator,” *IEEE Transactions on Electron Devices*, vol. 16, no. 1, pp. 64–77, Jan 1969.
[10] H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems*. Oxford University Press (OUP), Jan 2007.
[11] A. J. Bennett, P. Atkinson, P. See, M. B. Ward, R. M. Stevenson, Z. L. Yuan, D. C. Unitt, D. J. P. Ellis, K. Cooper, D. A. Ritchie, and et al., “Single-photon-emitting diodes: a review,” *Phys. Stat. Sol. (b)*, vol. 243, no. 14, pp. 3730–3740, Nov 2006.