

GPU Computing of Quantum Dot Infrared Photodetectors

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Abstract—In this paper we present physics based mathematical models and numerical methods for fast GPU based simulations of advanced Quantum Dot Infrared Photodetectors based on new Quantum Dot technology (QDIP-NT). Details of successful experience of CUDA-implementation for GPU-based parallelization of simulations of 3D QDIP-NT photodetector model are described, and results are analyzed and discussed.

Keywords- *Quantum Dot, Infrared Photodetector, New Technology, Parallelization, GPU, CUDA, TCAD.*

Many applications require sensitive detectors in the infrared (IR) frequency range and operating at moderate cooling and even room temperatures. The new type of quantum dots (QD) infrared photodetectors nanotechnology (QDIP-NT), are being developed with the suppressed photoelectron capture time and, in this way, increased responsivity and improved noise characteristics compared to previous generation of QDIPs [1,2]. This QDIP technology needs new advanced, accurate simulation methods and tools to support the development SWIR and LWIR technology based systems, based on QDIP.

QDIP simulation tools deal with multiphysics and multiscale problem. First, the IR sensors are based on the phenomenon of photoconductivity in which a material becomes more electrically conductive due to photocarriers created by electromagnetic radiation. Second, photocarriers contribute to the electric current until they recombine or are trapped by impurities and defects. Long photocarrier lifetime would substantially improve operation of electromagnetic sensors. Time scales for these processes vary from 1ps to 1ms (six orders).

QD nanostructures are considered as a promising candidate for improving the room-temperature optoelectronic devices due to expected controllable intra-dot kinetics related to electron transition between discrete QD levels [3-6]. These expectations were based on the “phonon bottleneck” concept, which assumes that the phonon-assisted bound-to-bound transitions are prohibited, unless the energy between two discrete levels matches to the phonon energy [7]. According to this concept, the intrinsic electron relaxation in quasi-1D nano-objects, such as QDs, was anticipated to be significantly slower than in 2D and 3D structures. However, the phonon bottleneck model completely ignores modification of electron states due to interaction effects, e.g. due to a finite width of electron energy levels. It is not surprising that the experimentally measured phonon-mediated electron relaxation turned out to be much faster than it is expected in the phonon bottleneck concept [8-9]. Recent investigations [10] unambiguously demonstrated that the actual intra-dot kinetics is completely opposite to what can be expected for weakly interacting electrons and phonons. In reality, strong coupling between electrons and longitudinal

optical (LO) phonons leads to formation of the polaron states, which decay due to the interaction of LO phonons with acoustical phonons. Such kinetics results in strong energy and temperature dependences of the electron relaxation. After numerous experiments with various QD structures, no true phonon bottleneck has been found [8-9]. Thus, the intra-dot electron relaxation at room temperatures turns out to be very fast and practically unmanageable.

At the same time, recent advances in nanotechnology lead to new fascinating possibilities to fabricate QD nanostructures with novel geometries, various combinations of QD planes, rows, and clusters with different heterostructures, e.g. [11]. This opens wide possibilities for controlling inter-dot kinetics [1-6]. Simulation of QDIP nanostructures can be considered as an efficient approach for analyzing and improving the QDIP device design and performance.

I. APPROACH TO GOVERN PHOTOELECTRONS INTER-DOT KINETICS

A. New QD Technology

The most effective and reliable way to govern photoelectrons inter-dot kinetics is to use potential barriers in specially engineered QD structures, which have been proposed and developed by Dr. Mitin team at University Buffalo, NY [4-6] (called QDIP-NT) to improve the inter-dot kinetics [6-9]. Potential barriers around QDs are always created, when electrons from dopants outside QDs fill the dots. As an example, Fig. 1 shows local potential barriers around single dots evenly distributed in QD planes (ordinary QD structures). These barriers are created by localized electrons in the dot and dopants in the interdot space [5-6]. To effectively suppress electron capture process, the barrier height should be at least three - four times larger than kT . Therefore, if a photodetector is designed for room temperatures, the local barriers should be ~ 0.1 eV and, as simple evaluations show, quantum dots should comprise ~ 10 electrons (large dots and high doping required).

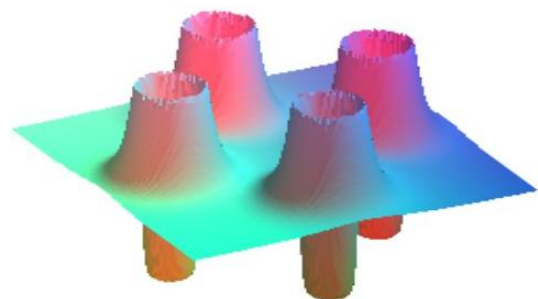


Fig. 1. Potential barriers around single dots in traditional QD structures with evenly distributed QDs

Fig. 2 represents the capture time as a function of electric field for three values of occupation. In order to contribute to the photocurrent, photo-excited carriers are driven by the applied bias. At small electric field, photocarriers are accelerated and the drift velocity linearly increases. When the electric field reaches a characteristic value, which is of the order of 10^3 V/cm, the electric field effectively heats the electrons. Electron heating increases an average energy of photoelectrons, which allows them to overcome potential barriers. Therefore, in the electric fields above $\sim 10^3$ V/cm the capture time decreases dramatically.

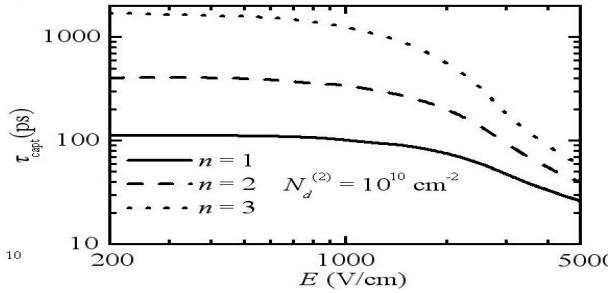


Fig. 2. Electrons capture time vs. electric field.

B. Problem description

For modeling of the photoelectron kinetics in these structures we use Monte-Carlo method approach, which includes electron scattering on acoustic, polar optical, and intervalley phonons. We use Γ -L-X model for simulation kinetics and transport in GaAs/AlGaAs structures with InAs dots [4]. Our results show that in small electric fields, the capture time exponentially increases with increasing of the height of the potential barrier V_m , Fig. 3. For QD structures with local barriers, the effect of the electric field can be understood in terms of the electron heating. The electric field increases the average energy (temperature) of carriers, so the barriers are less effective in preventing capture of hot electrons. Therefore, the capture time decreases as the electric field increases. The detector responsivity is proportional to the photoconductive gain g_{ph} , which is defined as a ratio of the photoelectron lifetime τ_ℓ to the transit time $\tau_{tr}=L/\mu E$. Summarizing this we would like to highlight that QDIPs can substantially outperform QWIPs due to manageable photocarrier kinetics, which can be controlled by potential barriers created by dot clusters. Modern technologies allow fabrication of various QD structures with specific manageable potential barriers.

II. QDIP SIMULATION WITH CUDA GPU TOOLS

The use of the barrier around the QD in QDIP can dramatically increase the carrier lifetime by many orders of magnitude, thus yielding the QDIP technology for room temperature. Optimal parameters of such device can be determined with 3D simulations which take large simulation times (days). Our GPU parallelization of the code is based on CUDA tools, to minimize efforts, and resulted in a dramatic acceleration (by 7X) while keeping high accuracy, and thus

reduced simulation time from days to hours. With further optimization, we have obtained additional 2X speedup (total 14X speedup). With new Fermi C2070 GPUs having very fast double-precision performance we expect extra 4X speedup.

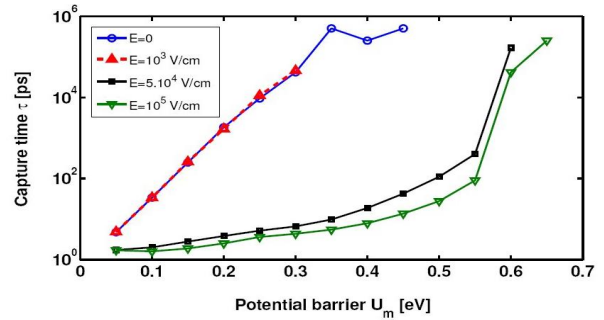


Fig. 3 Simulation of an electron capture by a quantum dots embedded in GaAs. Dot diameter 4.5 nm, separation 2 nm: average capture time vs. a height of the potential barrier U_m for different values of electric field. Simulated time 50 ps, time step 0.5 fs.

Table 1 Speed up factors for various problem sizes, fixed U_m

Number of Electrons	g77 serial code, Intel Xeon CPU	GPU parallel on Tesla GPU C1060	Speedup (vs original g77 code)
	Time (min)	Time (min)	X
10000	30.9	2.34	13.2
20000	61.8	4.46	13.9
40000	123.5	8.05	15.3
80000	247.2	15.50	15.9
160000	494.4	31.05	15.9

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