Exciton Dynamics and Charge Carrier Transport in SiGeSn based MQW devices

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***Abstract*—SiGeSn alloys have emerged as a versatile material system for integrated photonics, combining tunable bandgap engineering with strong light-matter interaction across the near- to mid-infrared spectrum. In this work, we investigate the dynamics of excitons and charge carriers in SiGeSn quantum-confined heterostructures using a tight-binding framework. The coupled equations of motion for electrons, holes, and excitons are solved in Liouville superoperator form, enabling a modular incorporation of optical excitation, relaxation, and boundary conditions via a density-matrix approach. The interplay between electronic and optical responses is explicitly modeled, with a coherent light-field source term driving the system out of equilibrium, including polarization dynamics and absorption. Our method has been applied to study non-equilibrium exciton dynamics in SiGeSn nanostructures and complements recent experimental work on MQW devices by reproducing key trends in the device performance, thereby offering a predictive and scalable framework for the design of integrated mid-infrared photonic components.**

***Index Terms*—SiGeSn heterostructures, exciton dynamics, tight-binding, density matrix, Liouville superoperator, photonics**

I. Introduction

Experimental studies have demonstrated improved LED performance in SiGeSn-based MQW structures compared to homojunction devices, due to enhanced electron confinement and efficient light emission, key for electrically pumped GeSn lasers [1]. In this work, we explore the potential of SiGeSn heterostructures for light-emitting applications. To this end, we develop a tight-binding-based simulation framework that captures both the electronic and optical properties of the structures, explicitly including Coulomb interactions between charge carriers. While similar modeling approaches have been applied, for instance to describe higher-harmonic generation in CdSe semiconductors [2], excitonic effects are often neglected in those studies.

We adopt a two-band, spin-less Hubbard formalism and employ localized Wannier functions. Phenomenological scattering, dephasing, and relaxation terms and the Coulomb interaction between excitons are taken into account. To solve the transient dynamics, we employ the master equation in Lindblad form. The observables studied include the electron and hole populations, the current, the absorption, and the exciton dynamics.

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II. Concept

The dynamics of the coupled electron-hole-photon system are governed by the following tight-binding Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_{em} + \hat{H}_C, \tag{1}$$

where each term represents a significant physical contribution:

- $\hat{H}_0$: The free tight-binding Hamiltonian, describing the kinetic energy and on-site potentials of electrons and holes.
- $\hat{H}_{\text{em}}$: The light-matter interaction in dipole approximation, coupling the electronic system to an external optical field.
- $\hat{H}_C$: The Coulomb interaction between electrons and holes.

The Heisenberg equation of motion for any operator $\hat{O}$ (e.g., excitonic $\hat{Y}_{ij}$, electron $\hat{C}_{ij}$, or hole $\hat{D}_{ij}$ operators) yields:

$$i\hbar\frac{d}{dt}\hat{O} = [\hat{O}, \hat{H}] = [\hat{O}, \hat{H}_0] + [\hat{O}, \hat{H}_{\text{em}}] + [\hat{O}, \hat{H}_C]. \tag{2}$$

By systematically evaluating these commutators as in [3], we derive a set of coupled nonlinear equations for the electronic and excitonic variables. To numerically solve this system, we use the master equation in Lindblad form

$$\frac{d}{dt}\vec{\Psi} = \mathcal{L}\vec{\Psi} + \vec{F}[\vec{\Psi}], \tag{3}$$

with $\mathcal{L}$ being the Liouville superoperator, containing the linear dynamics (coherent evolution, dissipation, and absorption) and $\vec{F}[\vec{\Psi}]$ capturing the nonlinear many-body effects, such as Coulomb renormalization and optical driving terms. The state vector $\vec{\Psi}$ contains the site-resolved coefficients of the tight-binding basis.

III. Numerical Evaluation

We first analyze a single quantum well (SQW) cell consisting of a GeSn well embedded in SiGeSn barriers, where the well width is varied to assess its influence on the optical properties. In a next step, several such cells are periodically arranged to form a multi-quantum well (MQW) structure,

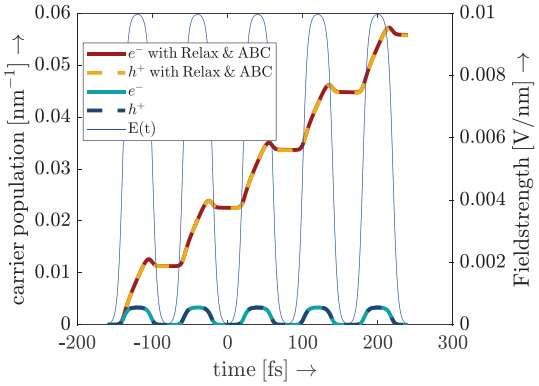

Fig. 1: Carrier excitation under a periodic modulated field. Relaxation and absorbing boundaries enable smooth carrier buildup and suppress reflections.

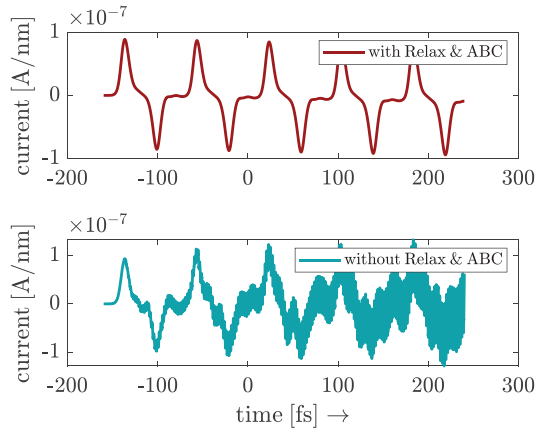

Fig. 2: Time evolution of the current density. The top panel demonstrates the effect of including relaxation and ABC, leading to a cleaner current flow.

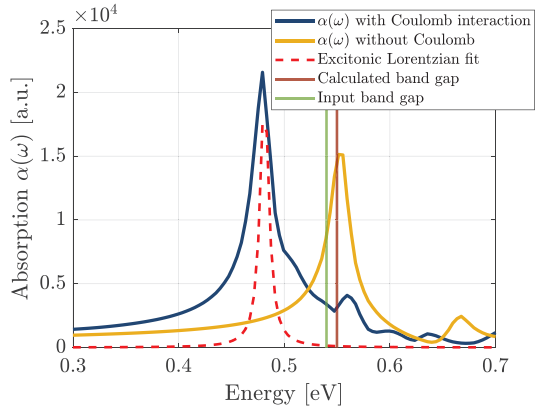

Fig. 3: Absorption spectra $\alpha(\omega)$ with (blue) and without (orange) Coulomb interaction, showing a redshift due to excitonic effects. The Lorentzian fit (red dashed) serves as a reference for both spectra. The red and green lines indicate the simulated and input band gaps, respectively.

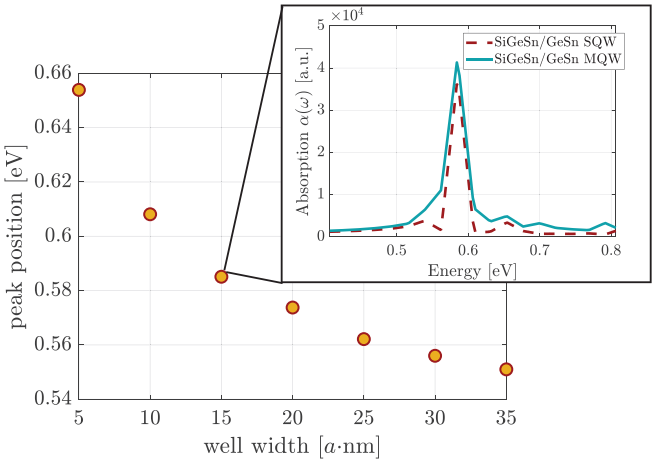

Fig. 4: Simulated absorption peak positions for varying well widths in SiGeSn/GeSn heterostructures. As the well width increases, the peak position approaches the bulk bandgap. The inset compares the normalized absorption spectrum of a single quantum well (SQW) and a multiple quantum well (MQW, 5 cells) structure at a well width of 15 nm, illustrating enhanced absorption in the MQW case.

allowing us to study the influence of inter-well coupling within the tight-binding framework. The first two Figs. 1 and 2 highlight the electronic structure and carrier dynamics by showing the charge carrier densities and the resulting current flow through the structure. In this context, we demonstrate the influence of relaxation terms and the use of an absorbing boundary condition (ABC) similar to [2] at the edges of the simulation domain, both of which significantly affect the system's behavior and the steady-state transport characteristics.

In contrast, Figs. 3 and 4 focus on the optical response of the system after excitation with an oscillating gaussian pulse by comparing the absorption spectra with and without Coulomb interaction. Additionally, a SQW is compared with a corresponding MQW structure composed of 5 cells to assess how quantum confinement and layer repetition influence absorption strength and spectral features.

IV. Discussion and Conclusion

We have developed a tight-binding-based simulation framework to study the electronic and optical properties of SiGeSn quantum well heterostructures, explicitly including Coulomb interaction and external fields. The model complements experimental studies by providing detailed insight into carrier dynamics and absorption processes across different well widths. Simulations reveal how relaxation and boundary effects influence carrier transport, while the optical response highlights excitonic shifts and enhanced absorption in MQW structures. These results establish a basis for the predictive design of efficient mid-infrared emitters using group-IV heterostructures.

References

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