# ULTRAFAST QUASI-BALLISTIC DYNAMICS OF LOW ENERGY PHOTOGENERATED ELECTRONS IN DOUBLE HETEROSTRUCTURES

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## Abstract

In a recent femtosecond pump-probe experiment involving the ballistic acceleration of bandedge photogenerated electrons in a GaAs-AlGaAs quantum well structure, a transient energy overshoot was observed. We attempt to analyse the experimental behaviour, by focussing on the transport issues and comprehensively modelling the internal carrier dynamics. Quantization effects on the phonon modes are included based on a hybrid macroscopic-microscopic approach. In addition, we allow for quantum corrections and, the possibility of carrier acceleration in response to electric fields during a "collision" event. Finally, space-charge effects modifying the time-dependent internal electric fields are also included. Our simulations are in good qualitative agreement with the actual experimental results. Based on a coupled Molecular Dynamics-Monte Carlo procedure we show that inclusion of two-dimensional electron-phonon scattering models is necessary, and use of bulk-like phonons yields unacceptable results.

## Introduction

With the advent of sub-picosecond lasers, it has now become possible to optically probe nonequilibrium carrier dynamics in arbitrary semiconductor structures, and direct experimental observation of phenomena that had hitherto been accessible only indirectly at best, has become possible. Despite the availability of raw experimental data however, its interpretation and analysis is not always easy since the observed response is collectively influenced by a number of on-going physical processes. For example, real space transfer, numerous quantum effects [1], complications of the band structure, and quantization effects on the phonon modes collectively make an impact on the overall transient dynamics. A more desirable situation for an accurate understanding of the internal physics, would be to focus on only a few individual processes and eliminate all remaining contributions. The recent femtosecond, optical experiments performed by Sha et al. [2] for the direct observation of ballistic electron transport in quantum well structures, are very effective in this regard. By virtue of the ultrashort time scales, many of the internal processes such as phonon amplification and carrier recombination are automatically turned off. In addition, by exciting carriers at the bandedge, complexities associated with the band structure, possible impact ionization, real space transfer and inter-subband transitions are also easily eliminated. The work of Sha et al. [2] is noteworthy since it also provides data which might help resolves some open points of discussion. For instance, there has been some question on how one incorporates phonon effects on the transport properties of a two-dimensional (2D) electron gas. Mismatch in the dispersion of optical phonon modes between the adjacent materials of such periodic structures is known to give rise to both confined and interface modes, and to modify the electron-phonon interaction. Though there exist a variety of models that could be used, here we show unambiguously that some of these approaches work poorly and are inappropriate for 2D transport modeling. Secondly, for many years it has been noted that the electron-

phonon interaction is not instantaneous, and that as a result an applied electric field can still accelerate carriers during a "collision" event. Here we shall show that the inclusion of the intra-collisional field effect and the breakdown of the Fermi golden-rule augments our ability to understand the experimental results. Finally, we demonstrate that space charge effects and the absence of carrier reinjection at the contact regions during the femtosecond time scale have an important influence on the field dependent dynamic response under conditions resembling those of the optical experiments.

We focus here on numerical simulations of the heating of cold electrons in a quantum well structure over sub-picosecond time scales. Apart from the electronic quantization effects, the role of the 2D phonons, the breakdown of Fermi golden-rule, time dependent space-charge effects, and the intra-collisional field effect (ICFE) will be comprehensively included. Besides simulating the field-dependent behaviour, numerical results under zero-bias conditions have also been included to focus on the optical phonon dominated electronic heating.

## Computational Scheme

As regards the model necessary for our calculations of the electron-phonon interaction, we have resorted here to a combination of macroscopic and approximate-microscopic approaches. Though a rigorous analysis of phonons in quantum well structures strictly requires a microscopic model [3] to yield the dispersion relations, the allowed vibrational modes, and the corresponding scattering potentials; its implementation is quite cumbersome and not well suited for transport calculations. Our choice in this regard, is guided by two significant developments from the recent past. First, as shown theoretically for the AlAs-GaAs system [3], the much simpler macroscopic slab model yields electronic scattering rates via interface phonons that are in good agreement with those derived from the rigorous microscopic approach. Secondly, experimental Raman data of transient hot phonon spectra [4] has also shown that the macroscopic approach is adequate for the describing the electron-interface phonon behaviour. In addition, the Raman spectroscopy results have clearly indicated that descriptions involving confined modes require at least analytical microscopic models for good accuracy. As a result, we use the macroscopic slab model based on the dielectric continuum theory for electron scattering via the symmetric/antisymmetric interface phonons, while our description of the confined mode scattering relies on the analytical microscopic approach of Huang and Zhu [5]. The Huang and Zhu model is more accurate over the entire range of phonon wavevectors, and satisfies both electrostatic and mechanical boundary conditions. Evaluation of the electron-phonon scattering rates is fairly straightforward and the details are given elsewhere [6].

Since application of the Fermi golden-rule may become questionable for simulations in the sub-picosecond regime [1] and some energy broadening is expected due to initial state decay; we resort to a Monte Carlo adaptation of the Barker approach [1] to include such aspects. As a result, the energy conserving delta function is replaced, within the framework of fully completed but non-instantaneous collisions, by an integral equation of the form:

$$\delta^{E,A} = \frac{1}{\pi\hbar}\int_0^{\infty} d\tau \exp\left(-\frac{\tau}{\Gamma}\right) \cos\left[\frac{\tau}{\hbar}(E' - E \pm \hbar\omega) \mp \frac{e\tau^2 F.q}{2m^*}\right] , \quad (1)$$

where T represents the state broadening against all scattering processes, F is the electric field, and **q** the phonon wavevector involved in the scattering process. By linearising the quadratic dependence of the cosine argument with the introduction of an effective collision duration time $\tau_c$, equation (1) can be integrated in a straightforward manner [6]. The net result is that the energy conserving delta function is replaced by a Lorentzian, which has to be used in making the energy selection of the final state after every scattering event for a Monte Carlo procedure. The final energy can then be obtained via a random number generation process [6]. In the present case, we have chosen to use the results of Lipavsky et al. [7] to define the collision duration time as: $\tau_c^{a,e} \approx h/(E \pm \hbar\omega)$, with E being the carrier kinetic energy.

## Results and Discussion

Based on the above description of the electron-phonon scattering, numerical simulations at 300 K were performed. In keeping with actual experiments [2], a 50 Å quantum well arising from a GaAs-$Al_{0.3}Ga_{0.7}As$ double heterostructure system was used for the computations. A 100 fs laser pulse was assumed to photogenerate carriers at the band-edge over a 50 μm x 50 μm area with a density of 2.5 x $10^{11}$ $cm^{-2}$. A two-subband coupled Ensemble Monte Carlo-Molecular Dynamics (EMC-MD) procedure [8] was employed. Only the heavy hole dynamics were taken into account, and transitions from the bound states into the AlGaAs energy continuum were ignored. This assumed absence of real space transfer is justified here as we shall presently show, and is also in accordance with actual experimental results.

Results of the time-dependent average electron energy obtained from a 2000-particle EMC-MD simulation at zero applied electric field are shown in Fig. 1. The curves obtained from two different phonon models, represent heating of the cold plasma through phonon absorption. The point of significance, is that increases in the average electron energy as represented by the lower curve, turn out to be in good quantitative agreement with the experimental data of Sha et al. [2] only when the 2D phonon model as described in the preceding section, is explicitly used for the calculations. With a bulk phonon model on the other hand, our simulations yield higher effective electron temperatures and unacceptably fast rise times as seen from the upper curve of Fig. 1. Our results therefore confirm the inadequacy of using the bulk Hamiltonian.

The more conventional bipolar Monte Carlo method (as opposed to the EMC-MD technique) was used to simulate the field-dependent energy transient at 16 kV/cm with 20,000 particles and a time step of 0.5 fs. The entire device structure was simulated, and transient variations of the net charge within the photoconductive gap was adequately taken into account. The ICFE and deviations from the Fermi golden-rule were implicitly included, carrier-carrier scattering was treated on a k-space formulation, and a Poisson solver with a mesh size of 125 Å was used to compute the time-dependent electric fields. Neumann boundary conditions were imposed to allow for charge variations, and electric fields at the two ends were continually updated at each time step by keeping track of the particle numbers exiting the simulation region. Given the sub-picosecond time scales of interest and the reverse biased conditions, we chose to ignore carrier reinjection at the contacts. Results for the average electron energies thus obtained are shown in Fig. 2. The overshoot structure is qualitatively similar to the actual experiments. The initial change in the energy is slow mainly due to the continuous generation of cold electron during the first 100 fs. The subsequent rapid increase is a combined result of quasi-ballistic motion, and phonon absorption. Consequent removal of the faster moving electrons, the phonon emission process, and a build up of the polarization fields reduces the average energies. The electron distribution functions obtained from the simulations is shown in Fig. 3 at the time instants of 100 fs and 250 fs. The minor bump appearing on the 100 fs curve is the signature of phonon absorption. Overall both curves exhibit a nearly thermal distribution and reveals an absence of real space transfer.

Besides the electrostatics, the energy overshoot is also influenced by quantum corrections and energy broadening effects. Due to deviations in the Fermi golden-rule, not all of the electrons lying close to the band-edge and undergoing a phonon absorption process, can be transferred into energy states above the emission threshold. Instead, a finite fraction of the scattered electrons could only be transferred into more energetic states by subsequent absorption; and the overall effect would amount to a reenforcement of the transient increase in the average electronic energy. Such behaviour is shown in Fig. 4, from EMC simulations of the time-dependent average electronic energy following a 20 fs bandedge laser excitation. The calculations were performed with and without the quantum corrections. One expects such an effect to be washed out for larger photoexcitation energies. Before closing, we mention that the present analysis has used a simple scalar potential. However, in actual experiments the propagating signals cannot cross the gap during the ultrashort time durations. A wave equation is therefore needed to fully describe the movement of the electromagnetic information inside the gap, and to take account of radiative losses as have experimentally been observed. A more refined simulation model to include such effects is in progress.

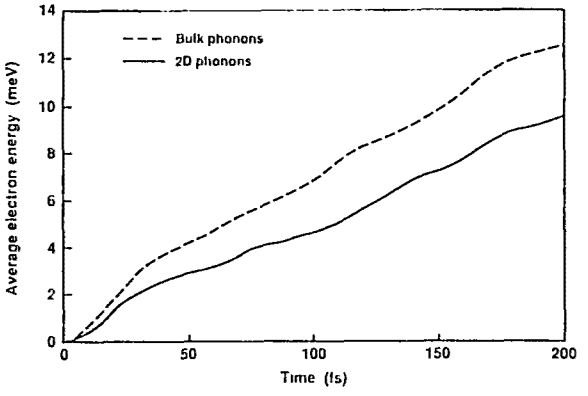


Fig. 1 Zero field EMC-MD simulations at 300K showing the temporal evolution of the average electron energy.

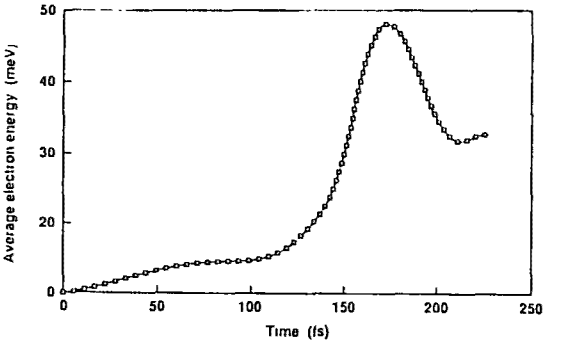


Fig. 2 Mean electron energy following a 100 fs bandedge laser pulse at an initial 16 kV/cm field.

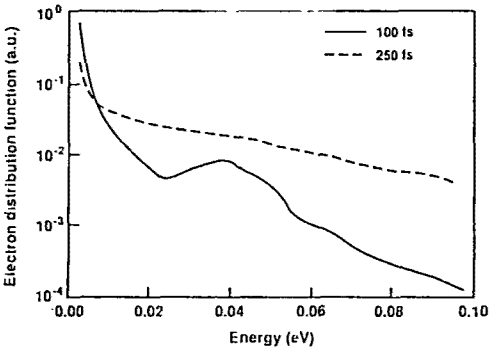


Fig. 3 Electron distributions at 100 fs and 250 fs following photogeneration for a 16 kV/cm initial electric field.

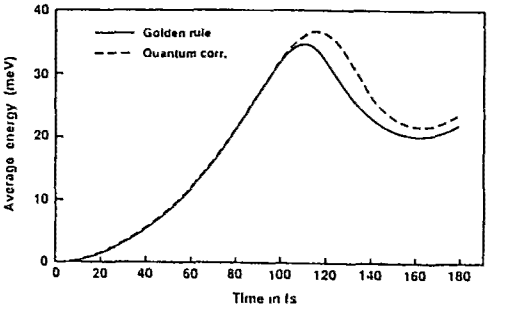


Fig. 4 Average electron energies with and without quantum corrections at 16 kV/cm and an 20 fs bandedge pulse.

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