Electrical Excitation of Surface Phonon-Polaritons in III-V Heterostructures: a Monte Carlo study

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Abstract. The surface phonon polaritons (SPP) excitation by hot electrons of an appropriate two-dimensional gas could make possible to implement an opto-electronic device emitting around 10 THz. To quantitatively assess the SPP emission by inter-subband electron relaxation in a GaAs/AlGaAs quantum well, accurate electron/SPP scattering rates have been included in a particle Multi-Subband Monte Carlo (MSMC) simulator. Our results suggest some possible optimizations to enhance the SPP emission in order to design new Tera-Hertz sources.

1. Introduction
Surface plasmons polaritons have been widely investigated and now offer the possibility of designing optoelectronic devices operating in the THz frequency range [1]. The same potential is expected for phonon polaritons in semiconductor structures and devices. Recently, phonon-polariton waves have been experimentally studied on the surface of SiC crystal [2], and infra-red emission of thermally excited SPPs has been observed in polar materials, by grating-induced diffraction [3]. This paper investigates an SPP excitation method by hot electrons inter-subband transitions in a 2DEG. An AlGaAs/GaAs quantum well heterostructure and the surface wave over the air/GaAs interface are studied. Within the Fermi golden rule, analytical expressions of SPP scattering rates are first derived using electromagnetic surface wave quantization and simplified SPP dispersion relation. A Multi-Subband Monte Carlo (MSMC) simulator [4] has been modified appropriately to consider these electron/SPP scattering rates. The most important scattering phenomena governing the transport properties have been considered, i.e. interaction with SPP, bulk polar optical phonons (POP) and acoustic phonons (AP). Our simulations provide an accurate evaluation of the number of SPP emitted per unit of time as well as their wave vector distribution.

2. SPP scattering rates
The surface phonon scattering model developed here for an air/semiconductor interface, as presented in Fig. 1, will be used as a first approximation in device simulations of Section 3. Consider an electron of wave vector \( K \) in the \( m \)th subband of a 2DEG. The transition from this state to the state \( K' \) in the subband \( m' \) via electron-phonon interaction is described by the coupling matrix \( M' (\sigma = -1 \text{ for phonon emission}, +1 \text{ for absorption}) \) whose square element can be expressed in the first order perturbation theory as [5]
where $\Lambda$ is the surface area of the 2DEG. The term $G(q_{//})$ in (1) is obtained via the quantization of the electromagnetic surface wave associated with an SPP and is expressed by

$$G(q_{//}) = \frac{\varepsilon_0 \omega^2}{2} \left[ \frac{1 + \frac{q_{//}^2}{\kappa_{1L}^2}}{\kappa_{2L}^2} \frac{d}{d\omega} \left( \omega \varepsilon(\omega) \right) - \frac{1}{\kappa_{1L}^2} \frac{q_{//}^2}{\kappa_{2L}^2} \right] \varepsilon(\omega) \left( \frac{q_{//}^2}{\kappa_{2L}^2} \right)$$

(2)

The SPP is defined by its angular frequency $\omega$, its in-plane wave vector $q_{//}$ and its normal absorption components $\kappa_{1(2)}$ characterizing the vanishing of the electric field in the first (second) material. The two considered materials are air (labelled by subscript 2) and semiconductor (subscript 1), thus only the GaAs dielectric function $\varepsilon(\omega)$ is involved [6]. In (1) $u$ and $u_z$ are the unit vector in SPP wave direction and the perpendicular unitary vector, respectively (see Fig. 2). The energy distribution of SPPs is described by the Bose-Einstein statistics $n_{q_{//}}$. The overlap integrals $Z_1$ and $Z_2$ are given by

$$Z_1 = \int e^{-\kappa_{1L} \xi^+ m (z)} \xi^{- m} (z) dz \quad Z_2 = \int \frac{1}{\kappa_{1L}} e^{-\kappa_{2L} \xi^+ m (z)} \xi^{- m} (z) dz$$

(3)

where $\xi^+ m (Z)$ is the electron envelope function for the subband $m$.

**Figure 1.** Electron/SPP scattering scheme

**Figure 2.** Structure of simulated device

The SPP dispersion is approximated by the step function $\omega(q_{//}) = \omega_{SPP} U(q - q_0)$, where $\omega_{SPP}$ is chosen as the asymptotic value of the SPP dispersion ($\hbar \omega_{SPP} = 36 \text{ meV}$) and $q_0$ is the wave vector limit value satisfying the surface resonance condition ($q_0 = 1.61 \times 10^6 \text{ m}^{-1}$). Integrating $M^\sigma$ over all possible final states gives the electron/SPP scattering rate $\lambda(E,m)$ for an electron of kinetic energy $E$ in subband $m$:

$$\lambda(E,m) = C_{SPP} \cdot \omega_{SPP} \int d\theta \cdot n_{q_{//}+\sigma/2} \left( 1 + 2\alpha(E + \sigma \hbar \omega_{SPP}) \right) \frac{\left| Z_{1(u,K + \sigma q_{//}Z_2 u_z,n)^2} \right|^2}{G(q_{//})}$$

(4)

where $C_{SPP} = e^2 / 4\pi m^*$, $\theta$ is the deviation angle, $e$ is the electron charge and $m^*$ is the electron effective mass corrected by a non-parabolicity coefficient $\alpha$. Only the $\Gamma$ valley of GaAs is considered here.
The resulting inter-subband and intra-subband SPP emission rates for the 1\textsuperscript{st} and 2\textsuperscript{nd} subbands in an AlGaAs/GaAs quantum well heterostructure at room temperature are plotted in figure 3. Figure 4 compares the most frequent SPP emission rate for electrons in the first subband with that of the most frequent emission of bulk polar optical phonons (POP) and acoustic phonons (AP). It is worth noting that the emission rate corresponding to inter-subband transition SPP\textsubscript{2-1} from the second to the first subband which generates an SPP with short wave vector is the only scattering rate that decreases when initial electron energy increases (fig. 3). It is also shown that for low energy electrons, SPP emission rates values are about one decade less than that of POP emission which is the dominant scattering mechanism in III-V materials. However, these two emission rates become similar at high energy.

![Figure 3](image1.png)  
**Figure 3.** SPP/electron intra-subband and inter-subband emission rates.

![Figure 4](image2.png)  
**Figure 4.** Scattering rate of most frequent AP, POP and SPP processes in the 1\textsuperscript{st} subband.

3. MSMC simulation results

To analyse the electronic transport and to assess the potentiality of hot electron to enhance the SPP emission, a Multi-Subband Monte Carlo simulator including SPP scattering rates was applied for the device presented in fig. 2. First, a 1D Schrödinger/Poisson simulation was performed along the $z$ axis to provide quantum energy levels and electron wave functions for the biased structure based on a typical AlGaAs/GaAs HEMT. These wave functions are used to calculate the SPP scattering rates within the model developed in Section 2. Frozen-field MSMC simulations were then performed. Such type of simulation solves the Boltzmann equation without any assumption on the distribution function, which actually allows a qualitative and quantitative analysis of electron/SPP interaction properties.

![Figure 5](image3.png)  
**Figure 5.** Number of SPP, POP and AP emitted per second and per surface area as function of electric field $E_y$, $\Delta E_{12}$ is fixed at $\hbar \omega_{SPP}$.

![Figure 6](image4.png)  
**Figure 6.** Spectrum of emitted SPP wave vector for $E_y = 1\text{kV/cm}$ and $\Delta E_{12} = \hbar \omega_{SPP}$. In inset: same spectrum for $\Delta E_{12} = 30 \text{meV}$.
The numbers of emitted phonons (SPP, POP and AP) per second and per unit area of surface as a function of the electric field in the transport direction are plotted in figure 5. Consistently with scattering rates of Fig. 4, the number of POP emissions is always less than one decade smaller than that of SPP emissions. However, because of decreasing POP emission rate at high energy, increasing the electric field is more favourable to the SPP emission than to the POP one.

To produce THz radiations, short wave vector SSPs may be collected by a grating structure at the top of the device. To evaluate this possibility the SPP wave vector distribution has been investigated together with its dependence on the energy difference $\Delta E_{12}$ between the 1st and 2nd subbands. Maximum of short wave vector SPP emission, useful for THz emission, is obtained for $\Delta E_{12}$ just equal to the SPP energy $\hbar \omega_{SPP} = 36 \text{meV}$ (fig. 6). For other values of $\Delta E_{12}$ (e.g. as in inset of fig. 6, for $\Delta E_{12} = 30 \text{meV}$), the most frequent scattering mechanism (not shown) is the intra subband band SPP emission (SPP_{1,1} in figure 3). This transition generates SPPs with wave vector on the order of magnitude of electron wave vectors i.e. equal to about $10^8 \text{m}^{-1}$. SPPs with short wave vector are more efficiently generated by electron transitions from 2nd to 1st subband. This scattering mechanism is enhanced for $\Delta E_{12} = \hbar \omega_{SPP}$. In this case, high electron kinetic energy is not necessary to emit SPPs because of decreasing SPP_{2,1} scattering rate (see Figure 3). This low wave vector phonon emission depends on $\Delta E_{12}$ which is controlled by the gate voltage. To make possible the THz radiation from SPPs of wave vector as close as possible to $10^8 \text{m}^{-1}$ the grating structure should be optimized with a period smaller than 50 nm. In this case, one can benefit from a strong intra-subband emission of SPPs by high energy electrons of the first subband.

4. Conclusion
Theoretical estimation of the emission of SPPs via intra- and inter-subband interactions in an AlGaAs/GaAs two-dimensional electron gas has been carried out using appropriate multi-subband Monte Carlo simulation. Our calculations show that SPP emissions are not negligible compared to other mechanisms of phonon emission, which supports the idea that electrically-induced SPPs have the potential to generate THz radiations. Our results also suggest that a device appropriately biased to favour the non-stationary transport of hot electrons may be helpful to generate a large amount of SPPs and thus to design an efficient THz source. The other key point is then the design of the diffraction grating structure which has to couple efficiently SPPs with photons. Further theoretical works are needed to model accurately the effects on SPP emission of the gate and of the material stack, including the presence of the additional grating structure. Next studies will focus on alternative materials and multi-interface structures to explore more deeply the potentialities of electronic SPP emission.

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