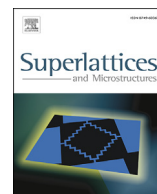




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## A study of the coupling between LO phonons and plasmons in InP p-i-n diodes

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### ARTICLE INFO

#### Article history:

Received 14 November 2016

Received in revised form 17 January 2017

Accepted 17 January 2017

Available online 30 January 2017

#### Keywords:

Collective oscillations

Coupling

LO phonon

Plasmon

THz emission

InP

p-i-n diodes

### ABSTRACT

This paper reports a study investigating the coupling between longitudinal optical (LO) phonons and plasmons in InP p-i-n diodes by a numerical simulation. A significant change is observed in the Fourier transform spectra of transient electric field when taking the coupling into account. The findings show two separate peaks instead of a single plasma peak as for non-coupling case. In addition, the bulk-like dispersion relations of the frequencies of those two peaks on the carrier density are found. Therefore, it is proposed that those behaviors manifest the LO phonon-plasmon coupling in the diodes. Also, there is evidence of the peak clipping by the diode itself, a phenomenon not being seen in the bulk InP semiconductor.

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## 1. Introduction

Semiconductor nanostructures have attracted considerable attention as their nanoscale sizes can potentially improve the technologies [1–5]. Moreover, the development of the ultrashort pulse lasers has revealed velocity overshoot phenomena and coherent oscillations within nanostructures [6,7]. Terahertz (THz) radiations, which can rise from those two phenomena, have shown promising applications in imaging technologies, especially in THz imaging and spectroscopy [8,9]. Nonetheless, due to the high costs of current THz devices, physicists have extensively quested for alternative THz radiation sources [10–16], one of which is plasma oscillation [17–19].

InP p-i-n diodes may also possess a promising THz source from plasma oscillation [12,13]. To stabilize THz equipment, plasma frequency should be strictly monitored, which is hardly possible since it is a time-varying function of carrier density. Moreover, when plasmon frequency is close to that of LO phonon, the coupling between them can be seen. It is imperative to investigate how the coupling affects such diode properties as optical spectra because coupling interaction can transform any spectrum of diodes, both in intensity and in spectrum components. Hence, more related works in InP p-i-n diodes are needed to find out those changes and to better control spectrum.

To study semiconductor devices, many theoretical approaches, including Green's function [20], density functional method [21], Boltzmann's equation, and drift-diffusion model have been utilized [22]. Especially, self-consistent ensemble Monte-

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Carlo (EMC) method with additional advantages of high accuracy and stability has been widely used [22–31]. This is a semi-classical approach in which carrier dynamics is found from Newton's equations of motion while scattering rates are determined by Fermi's golden rule of quantum theory. This semi-classical approach is proved to be suitable for the simulation of submicron devices [22,26–28]. Moreover, this EMC method has been adapted to simulate various structures emitting THz radiation, as in works carried out by Johnston's group [28–30], and Tomizawa's group [22–25]. It is obviously seen that both groups basically stay on the same background, that is self-consistent EMC method. Moreover, the injection and distribution of thermalized and photoexcited carriers at the earliest stage of the simulation are similar. However, there are minor differences in two groups' approaches, such as kinds of scatterings used in the simulation, ways to estimate THz electric field, and numerical methods for solving Poisson's equation [25,28].

In this paper, interaction between LO phonons and plasmons in InP p-i-n diodes is characterized by an adapted Monte-Carlo simulation, following Tomizawa's approach [22–25]. In terms of calculation, various scatterings of impurities, acoustic phonons, non-polar and polar optical phonons, and plasmons were taken into consideration. To monitor ultrafast carrier dynamics in p-i-n diode, the time evolution of the distribution of carriers [31] was taken into account according to the experimental profile of laser pulses [12,13] in Monte-Carlo program. It is assumed that the usual 3-valleys model for conduction band in which each valley is approximated by a hyperbolic dispersion relation. Similar dispersion relation for the valence band is also used. At the beginning, all electrons stay in  $\Gamma$ -valley. Electrons will transfer from  $\Gamma$ -valley to L- and then to X-valleys when their energies increase to proper values. Equation of motion of LO phonons is first solved to find lattice polarization charge. Lattice polarization charge is then added to charge-density term of Poisson's equation to find transient electric field. Two coupled peaks are seen in the Fourier transform spectra of transient electric field when taking the coupling into account, instead of a single plasma peak as for non-coupling case. In the subsequent sections, the model and method of calculation is described in section 2, and the Monte-Carlo analysis of the interaction in InP p-i-n diodes is presented in section 3. In section 4, a summary of our approach and key results is provided.

## 2. Model and method of calculation

This study focuses on the coupling between LO phonons and plasmons in InP p-i-n diodes. As mentioned above, the coupling can transform any spectrum of the diodes and thus, the role of the coupling can be displayed. It is expected to show the role of the coupling through an analysis of the emission spectra of collective oscillations. The emission spectra of collective oscillations can be deduced from transient electric field as explained below. When there is no biased (external) field, transient electric field includes only built-in field. Built-in field is conducted by all electric charges in a device including free electrons and holes as well as positive and negative ions. Built-in field in this case mostly results from photoexcited carriers because there is only a small amount of doped particles. Therefore, the emission spectra of collective oscillations can be found through the Fourier transform of transient electric field under zero bias voltage. The Fourier transform is carried out with fast Fourier transform technique, and moving average filter to cut random noise in time domain signals, as well as Hamming window filter to raise the resolution of frequency spectrum [32].

In order to perform calculations, it is necessary to develop a model of diodes. It is assumed that InP p-i-n diodes contain an intrinsic (i)-layer surrounded by a p-layer and an n-layer, see Fig. 1 [33]. The  $d_i$ ,  $d_p$ , and  $d_n$  denote the thickness of those layers, respectively. The donors and acceptors are distributed according to Gaussian form in perpendicular direction to the surface of doping layers [33]. Photoexcited electrons and holes are simulated to be injected and distributed inside diodes according to experimental setup [12,13]. Carrier density is calculated as a time-varying function of laser parameters [31]. Obviously, photon energy has to be over material bandgap to excite those photocarriers into conduction and valence band. When excited by ultrashort laser pulses, electrons and holes conduct a coherent collective oscillation inside diodes, namely, coherent plasma oscillation.

LO phonon-plasmon coupling occurs in a bulk semiconductor when plasma frequency approaches the frequency of LO phonons, and the frequencies of two coupled branches ( $L_+$  and  $L_-$ ) are given by Ref. [34]

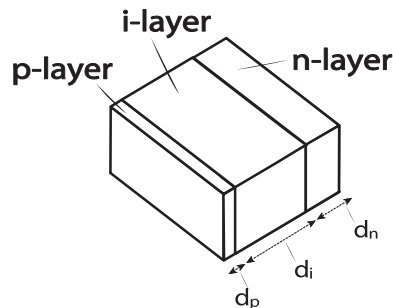


Fig. 1. Illustrative view of an InP p-i-n diode.

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