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2004 J. Phys.: Condens. Matter 16 4221

(http://iopscience.iop.org/0953-8984/16/24/004)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **16** (2004) 4221–4232 PII: S0953-8984(04)73764-9

Coupling of intrinsic localized modes in doped polar semiconductors with plasmons

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Received 22 December 2003
Published 4 June 2004
Online at stacks.iop.org/JPhysCM/16/4221
doi:10.1088/0953-8984/16/24/004

Abstract

We present a detailed analysis of the interaction between intrinsic localized modes and plasmons in a doped polar semiconductor. The investigation has been performed for an anharmonic one-dimensional diatomic lattice with alternating interactions coupling successive neighbours. The system simulates a row of atoms in the ⟨111⟩ direction of a III–V semiconductor. Specific calculations have been performed for GaN, because it has a large gap between the acoustic and optical phonon branches. The calculations of the intrinsic localized modes have been performed by using two-body potentials to describe the interactions. We have used the rotating wave approximation and we have found the intrinsic localized modes in the phonon gap. The interaction with the plasmon has been studied by adding to the equations of motion the alternating electric field which is related to the electron density of the plasmons. We obtain an expression for the electric dynamical polarization associated with the intrinsic localized modes and with the plasmons. We derive an expression for the dielectric function of the coupled system. The zeros of the dielectric function give the frequency of the combined modes. We have found two regimes in which combined modes are possible. One is related to small anharmonicity of the potential. The combined mode has a frequency above the top of the optical branch and can be explained in terms of the theory of the harmonic dielectric response of polar lattice vibrations. The second regime is related to high anharmonicity. The combined modes exist only for a finite slab. We show that on increasing the anharmonicity, i.e. the amplitude of the intrinsic localized mode, the width of the slab increases. The frequency of the combined mode is inside the phonon gap. We have also studied the dynamical stability of these modes.

1. Introduction

In recent years considerable theoretical attention has been devoted to modes referred to as intrinsic localized modes (ILMs) [1]. These modes are stabilized in a translationally invariant lattice by the anharmonicity of the crystal, thus displacements are similar to those produced by impurity atoms in a harmonic crystal. These modes were found in a one-dimensional monoatomic lattice, by using second and quartic force constants, to lie above the maximum of the phonon acoustic branch. The inclusion of a cubic force constant lowers their frequencies. With increasing amplitude of the cubic coefficients the frequency of these modes goes, for a Bravais lattice, into the continuum and the localized modes become unstable. The study of diatomic chains with a realistic potential, which includes anharmonicity to all orders, demonstrates that the ILMs appear only in the gap between the acoustic and the optical branches [2]. It has also been shown, for a three-dimensional diatomic system, that the use of the full potential gives rise to ILMs inside the gap. Recently ILMs due to anharmonicity have been observed in crystalline arrays of charged linear chains of PtCl with resonant Raman scattering [3]. Intrinsic localized spin modes have been generated and detected in quasi-one-dimensional biaxial antiferromagnets in the spin wave gap [4]. In the present paper we consider a diatomic chain with two alternating masses which represents a row of atoms along the $\langle 111 \rangle$ direction of a zinc-blende structure. In particular we will investigate a row of GaN which has a relatively large vibrational gap. In a previous paper [5] we have studied the ILMs of GaN by using a two-body potential to describe the interactions among all particles in the zinc-blende structure. These intrinsic modes have frequencies lying in the gap. The chain of zinc-blende structure has no centre of inversion, so we cannot classify the modes as even or odd. However, these modes will be classified as quasi-even and quasi-odd to indicate the relation to the corresponding modes when a centre of inversion exists.

In this work we present a study of the coupling of bulk intrinsic localized modes in a doped polar semiconductor with plasmons. In the long wavelength plasmon the dominant interaction is the Coulomb interaction between electrons, so we neglect the electron–phonon interaction and the scattering/trapping of a single electron by the breather, which lead to highly localized electronic states. In our scheme the conduction electrons, because of the excitation of the plasmon, are producing an uniform AC electric field of frequency ω_p lying in the phonon gap or above. We consider the action of this electric field on the stationary ILM arising from the bulk optical branch. We obtain expressions for the dynamic electric polarization associated with the plasmon and with the ILM. We then obtain an expression for the dielectric function of the coupled system. The zeros of the dielectric function yield the frequency of the combined modes.

In section 2 we discuss the interatomic potential and the numeric procedure used to solve the nonlinear system of equations of motion to determine the ILMs. Here we define the limit of small and large anharmonicity in terms of the maximum amplitude of the ILM. This distinction will be useful for discussing the interaction of the ILM with the plasmons. The interaction with the plasmon is obtained by adding an electric field to the equations of motion. In the same section we will show how the electric field is connected with the plasma oscillations and with the doping of the semiconductor. In section 3 we will discuss the case of small anharmonicity. We will present an expression for the polarization of the coupled modes. By varying the electron plasma frequency we will determine the frequency of the longitudinal combined mode which produces the vanishing of the electric displacement field D, which corresponds to the vanishing of the dielectric function. We then compare these results with those obtained with the harmonic theory of the dielectric response of polar lattice vibrations. The dynamical stability analysis of the modes is discussed in section 4.

A discussion of strong anharmonicity will be given in section 5, where we will also treat the case of a thin slab. In the final section 6 we will draw the conclusions.

2. Theory

We consider a one-dimensional chain with two alternating masses of Ga and N. A light atom of N is taken at the origin of the unit cell. The N atom is strongly bonded to the heavy Ga atom of the basis, which in turn is weakly bonded to the previous N atom. We describe the strong interaction with the potential of Zapol *et al* [6], containing a repulsive exponential part and a Coulombic attractive part, constructed to match bulk properties of the three-dimensional GaN. To describe the weak interaction of our one-dimensional system we use the same form of the potential, but we change the parameters of the long range Coulomb interaction in such a way that an expansion to second order in the displacements around its minimum can be used to reproduce the longitudinal acoustic (LA) and optical (LO) branches in the $\langle 111 \rangle$ direction. Considering nearest neighbours interactions, the equation of motion of the particle at the lattice site l in the presence of an electric field $\vec{\mathcal{E}}$ due to the plasmon is

$$m_l \ddot{u}_l = V'_{l+1}(u_{l+1} - u_l) - V'_l(u_l - u_{l-1}) + e^* \mathcal{E}(-1)^{l+1} \tag{1}$$

where u_l is the displacement of atom l and $V_l(u_{l+1} - u_l)$ is the interaction potential of neighbouring atoms. For l even, $V_l(u_l - u_{l-1})$ is the potential relative to the strong interaction and m_l is the mass of the light atom. For l odd, $V_{l+1}(u_{l+1} - u_l)$ is the weak potential and m_l is the mass of the heavy atom. The prime means a partial derivative with respect to the atomic displacements. e^* is the effective charge of the polar crystal and $\mathcal{E}$ is an alternating electric field. We first determine the ILMs. To this purpose we set the electric field equal to zero. Here we consider quasi-odd gap modes which give the maximum of polarization in each cell. We use the rotating wave approximation (RWA), so that the equations of motion represent oscillators which oscillate in time with a frequency ω. To apply the RWA to equation (1) we Fourier transform the potential, retaining the zero order term and the first order term in $\cos(\omega t)$. The details of the Fourier transform of the potential are given in the paper of Kiselev *et al* [7]. We look for stationary solutions of the type

$$u_l = a_0 A(\xi_l \cos(\omega t) + \phi_l) \tag{2}$$

where a_0 is equal to 1 Å. A is the maximum amplitude of the mode; the normalized vibrational amplitude ξ_l and the static displacement ϕ_l related to the local expansion of the anharmonic lattice are independent of time. We note that, on expanding in power series the potential of equation (1), the harmonic approximation is recovered for $A = 0.0$. The nth derivative of the potential contains the term A^{n-1}. For this reason the parameter A is governing the anharmonicity of the potential. Substituting equation (2) in (1) and making the RWA we obtain a system of coupled equations connecting the static and dynamical displacements to the applied electric field. To solve this system we use a routine based on the Newton scaled gradient method. We start with three atoms and an initial guess for the displacements of the quasi-odd solution ($\xi_0 = 1$, $\phi_0 = 0$, $\xi_1 = \xi_{-1}$, $\phi_1 = \phi_{-1} = 0$). The routine then determines the solution through an iterative procedure. One atom is then added to each end of the chain and the calculation of the displacements is repeated. The iterative procedure is continued up to 400 atoms. The addition at step n of two atoms acts as a perturbation on the chain. If the iterative perturbation does not destroy the mode, we consider the mode to be numerically stable. The dynamical stability of these modes is discussed in section 4. The frequency of the stationary solutions versus the maximum amplitude A is drawn in figure 1. The frequency is well resolved from the bottom of the optical phonon branch for amplitude $A > 0.10$, the

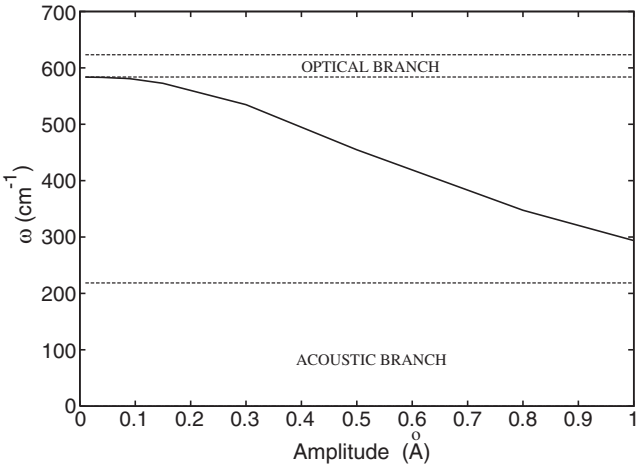

Figure 1. Frequency of the ILM in undoped GaN versus dynamical displacement amplitude.

ILM is well localized and we call this region the high anharmonicity region. In the range $0.001 < A < 0.10$, that we call the low anharmonicity region, the localized mode is already present, but the small amplitude give rise to a small anharmonic frequency shift from the bottom of the optical branch. As shown in the next sections, the electric field will produce different behaviour of the combined mode in the two regions.

We now discuss how the electric field $\vec{\mathcal{E}}$ is associated with the plasma frequency of the free carriers due to donors. The electric field is determined by the doping of the crystal. For the minimum doping here considered, $n_0 = 5.0 \times 10^{17}$ cm^{-3}, the electric field is $\mathcal{E} = 3.0 \times 10^7$ V m^{-1}, corresponding to a plasma frequency $\omega_p = 190$ cm^{-1}, while for the maximum doping investigated, $n_0 = 1.0 \times 10^{20}$ cm^{-3}, the electric field is $\mathcal{E} = 3.0 \times 10^9$ V m^{-1}, corresponding to a plasma frequency $\omega_p = 3000$ cm^{-1}. In this range of values the electric field cannot be considered as a small perturbation. We use international units in the following.

Let the static and dynamic electron concentrations be n_0 and n. We use the Maxwell equation

$$\vec{\nabla} \cdot \vec{\mathcal{E}} = \frac{e(n - n_0)}{\epsilon_0} \tag{3}$$

and the equation of continuity which is, when linearized,

$$\frac{\partial n}{\partial t} + n_0 \vec{\nabla} \cdot \vec{v} = 0. \tag{4}$$

We assume

$$\begin{aligned} \vec{\mathcal{E}} &= \vec{\mathcal{E}}_0 \mathrm{e}^{\mathrm{i}(\vec{k}\cdot\vec{r} - \omega t)}, \\ \vec{v} &= -\mathrm{i}\vec{v}_0 \mathrm{e}^{\mathrm{i}(\vec{k}\cdot\vec{r} - \omega t)}, \\ \Delta n &= n - n_0 = \Delta n_0 \mathrm{e}^{\mathrm{i}(\vec{k}\cdot\vec{r} - \omega t)}. \end{aligned} \tag{5}$$

To have a longitudinal mode we take $\vec{k} \parallel \vec{v}$ and $\vec{k} \parallel \vec{\mathcal{E}}$. Then the Maxwell equation and the equation of continuity become

$$\mathrm{i}\vec{k} \cdot \vec{\mathcal{E}}_0 = \frac{e}{\epsilon_0} \Delta n_0, \tag{6}$$

$$-\mathrm{i}\omega \Delta n_0 + n_0 \vec{k} \cdot \vec{v}_0 = 0. \tag{7}$$

For the longitudinal mode we obtain the following relation between the electric field and the electron velocity:

$$\vec{\mathcal{E}}_0 = \frac{en_0}{\epsilon_0\omega}\vec{v}_0. \tag{8}$$

We take the free carrier velocity and frequency as

$$v_0 = v_{\mathrm{F}} = \frac{\hbar}{m^*}\left(3\pi^2 n_0\right)^{1/3} \tag{9}$$

$$\omega = \omega_{\mathrm{p}} = \left(\frac{n_0 e^2}{m^*\epsilon_0\epsilon_\infty}\right)^{1/2} \tag{10}$$

where ϵ_0 is the vacuum dielectric constant, ϵ_∞ is the dielectric constant at frequencies high compared to the optical phonons frequencies, and m^* is the effective mass of the free carriers. With simple steps we get the desired relation between the electric field $\mathcal{E}_0$ and the plasma frequency ω_{p}:

$$\mathcal{E}_0 = \hbar\left(m^*\epsilon_0 3\pi^2\right)^{1/3}\epsilon_\infty^{4/3}\left(\frac{\omega_{\mathrm{p}}}{e}\right)^{5/3}. \tag{11}$$

Having evaluated the intrinsic localized modes which are located in the gap of the semiconductor, we switch on the electric field $\vec{\mathcal{E}}$ to determine the coupling between the ILMs and the plasmon. Now we take $\vec{\mathcal{E}} = \vec{\mathcal{E}}_0\cos(\omega t)$.

3. Weak anharmonicity

The case of weak anharmonicity corresponds to the condition $A \ll 0.10$, so that the potential in equation (1) is close to be harmonic. However, the electric field generated by the plasmon is not related to the value of A. To better clarify the discussion we start from the dielectric response of polar lattice vibrations for a linear chain in the harmonic approximation. In the case of an optical phonon the two atoms in the unit cell vibrate against one another and produce an electric dipole moment.

The total dynamical polarization is

$$\vec{P} = \sum_i^N \frac{e^*(\vec{u}_i^+ - \vec{u}_i^-)}{V} + \epsilon_0(\epsilon_\infty - 1)\vec{\mathcal{E}} \tag{12}$$

where N is the number of unit cells, $\vec{u}_i^+$ and $\vec{u}_i^-$ are the dynamical displacements of the positive and negative ions, respectively, of the ith cell, and V is the volume of the crystal. For the optical phonons of long wavelength the dipole moments of the various unit cells are in phase and are all equal, so that equation (12) becomes

$$\vec{P} = \frac{Ne^*\vec{u}}{V} + \epsilon_0(\epsilon_\infty - 1)\vec{\mathcal{E}} \tag{13}$$

where $\vec{u} = \vec{u}_i^+ - \vec{u}_i^-$ is the relative displacement of the two atoms in the unit cell. Writing equation (1) for atom $l = 0$ and atom $l = 1$ in the harmonic approximation in terms of the second order force constants k_2 for the strong interaction and $\bar{k}_2$ for the weak interaction, we obtain the following equation for the relative displacement $\vec{u}$:

$$\mu\ddot{\vec{u}} + (k_2 + \bar{k}_2)\vec{u} = e^*\vec{\mathcal{E}} \tag{14}$$

where μ is the reduced mass of the atoms in the unit cell and $\omega_{\max} = \sqrt{(k_2 + \bar{k}_2)/\mu}$ is the maximum frequency of the optical phonons. Fourier transforming we get

$$\vec{u} = \frac{e^*/\mu}{\omega_{\max}^2 - \omega^2}\vec{\mathcal{E}}. \tag{15}$$

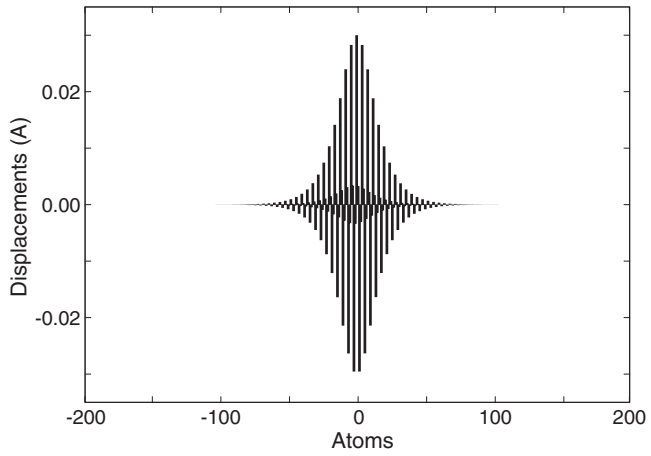

Figure 2. Dynamical displacement patterns of the ILM mode for $A = 0.03$ without electric field applied. The reference atom at site $l = 0$ is a light mass atom.

On inserting equation (15) in (12), the dielectric function $\epsilon(\omega)$ turns out to be

$$\epsilon(\omega) = \epsilon_\infty + \frac{e^{*2}/\mu V_0 \epsilon_0}{\omega_{\max}^2 - \omega^2} \tag{16}$$

where V_0 is the volume of the unit cell. The zero of the dielectric function $\epsilon(\omega)$ gives the frequency of the longitudinal mode, that we call ω_{LO}, and which is the analogous of the plasmon frequency produced by the electrons:

$$\omega_{\mathrm{LO}}^2 = \omega_{\max}^2 + \frac{e^{*2}}{\mu V_0 \epsilon_0 \epsilon_\infty}. \tag{17}$$

We note, from this equation, that the frequency of this longitudinal mode is above the maximum frequency of the optical branch. For $\omega = \omega_{\mathrm{LO}}$ equation (15) becomes

$$\vec{u} = -\frac{\mu V_0 \epsilon_0 \epsilon_\infty}{e^*} \vec{\mathcal{E}} \tag{18}$$

and $\vec{u}$ has the opposite sign to $\vec{\mathcal{E}}$. This gives a negative polarization which is necessary to fulfil the condition $\vec{D} = \epsilon_0 \vec{\mathcal{E}} + \vec{P} = 0$ or equivalently $\epsilon(\omega_{\mathrm{LO}}) = 0$.

With this in mind, we discuss the results of the calculations in the case of low anharmonicity. We start by evaluating the intrinsic localized mode with equation (1) without the electric field. In figure 2 the dynamical displacement pattern of the quasi-odd mode is presented for $A = 0.03$. The static displacements ϕ_l are negligible and are not presented. For small values of the anharmonicity the localized mode is spread over a hundred atoms and has a frequency located in the gap, but very close to the bottom of the optical branch, as shown in figure 1. We now solve equation (1) with the electric field and we call the solutions obtained mixed modes. Results obtained for the frequencies of the mixed modes versus the electric field defined by equation (11) are presented in figure 3 for different values of A. For small values of A, up to $A = 0.10$, the mixed mode is above the maximum of the optical branch, while for values of $A > 0.25$ the mode is always in the gap. There is an intermediate region, $0.10 < A < 0.25$, where the frequency of the mode can be both in the gap or over the optical branch: for small values of the electric field the mode is in the gap, then merges in the optical branch, and for larger values of the field goes over the top.

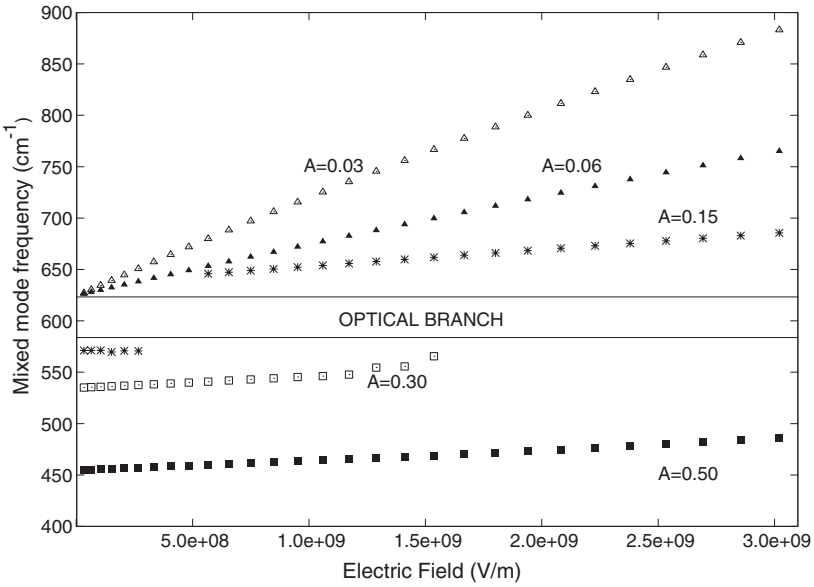

Figure 3. Frequency of the mixed modes versus electric field for different values of A. The range of the electric field is related to the doping. The range investigated goes from $\mathcal{E} = 3.0 \times 10^7$ V m^{-1}, corresponding to a plasma frequency $\omega_p = 190$ cm^{-1}, to $\mathcal{E} = 3.0 \times 10^9$ V m^{-1}, corresponding to a plasma frequency $\omega_p = 3000$ cm^{-1}.

We start by discussing the case of small values of A. In the equations of motion (1) the electric field term dominates the anharmonic terms and the displacement pattern loses the spatial localization and acquires a form similar to that of the optical phonons of long wavelength, the relative displacement of the ions in the unit cell being the same for all the cells of the crystal.

We name for convenience in the following as 'combined mode' the mixed mode which fulfils the condition $\epsilon(\omega) = 0$. The plasma frequency, i.e. the electric field, namely the doping density which satisfies the condition $\epsilon(\omega) = 0$ at a given value of amplitude A, is obtained numerically from the calculation of the dielectric function in the investigated range of highly doped GaN [8] with n_0 ranging from 5.0×10^{17} cm^{-3} to 1.0×10^{20} cm^{-3}. For each value of ω_p of figure 4 we evaluate the displacement pattern and the mixed mode frequency. Then by using equation (12) we evaluate the polarization $\vec{P}$ and the dielectric function $\epsilon(\omega)$ shown in figure 5. The frequency of the combined mode that fulfils $\vec{P} = -\epsilon_0 \vec{\mathcal{E}}$ is the frequency that we are seeking. In figures 4 and 5 the arrows indicate the plasma frequencies which fulfil the condition $\epsilon(\omega) = 0$ for the different values of the amplitude A. We discuss the case $A = 0.03$. The value of $\omega_p = 2055$ cm^{-1} gives the combined mode frequency $\omega_L = 772.6$ cm^{-1} corresponding to $\epsilon(\omega_L) = 0$, which is close to the exact value of equation (17) which is $\omega_{LO} = 772.3$ cm^{-1}, evaluated using the second order force constants derived from our full potential. This indicates that the case of small anharmonicity, which on the one hand produces an ILM in undoped GaN, on the other hand can be treated with the harmonic theory previously outlined in doped GaN when interacting with a plasmon. We further prove this statement for some different values of A. To keep fixed the value of ω_L one sees from equation (18) and from equation (11) that the ratio $u/\omega_p^{5/3}$ should remain constant. This is rather well verified in figure 4 for $A = 0.01$, 0.02 and 0.03. In conclusion, in the case of small anharmonicity the combined mode is mainly determined by the plasmon normal mode.

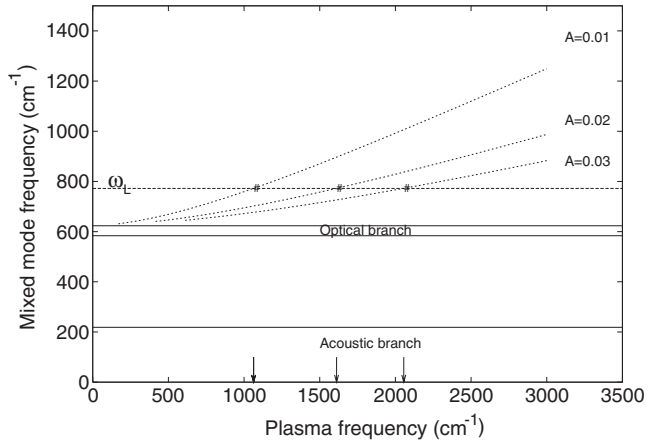

Figure 4. Frequency of the mixed modes versus plasma frequency. The symbol # indicates the 'combined mode' frequency which fulfils the condition $\epsilon(\omega) = 0$. The arrows indicate the corresponding plasma frequencies: $\omega_p = 1063\ \mathrm{cm}^{-1}$ for $A = 0.01$, $\omega_p = 1611\ \mathrm{cm}^{-1}$ for $A = 0.02$, $\omega_p = 2055\ \mathrm{cm}^{-1}$ for $A = 0.03$.

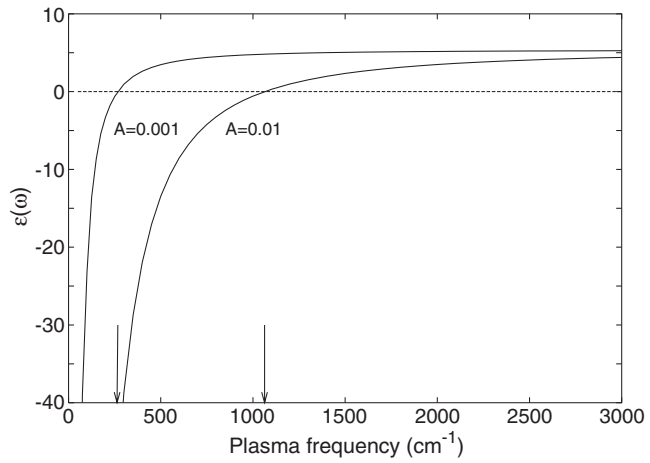

Figure 5. Dielectric function versus the plasma frequency. The arrows indicate the fulfilment of the condition $\epsilon(\omega) = 0$ for the two different values of A: $\omega_p = 267\ \mathrm{cm}^{-1}$ for $A = 0.001$, $\omega_p = 1063\ \mathrm{cm}^{-1}$ for $A = 0.01$.

4. Dynamical stability analysis

We have studied the dynamical stability of the stationary modes found in the previous section, assuming a displacement of the atom at site l as

$$w_l(t) = u_l(t) + \epsilon_l(t) = a_0 A(\xi_l \cos(\omega t) + \phi_l) + \epsilon_l(t) \tag{19}$$

where the perturbation $\epsilon_l(t)$ is small compared with $u_l(t)$. We have evaluated the force acting on the atom at site l to first order in the perturbation $\epsilon_l(t)$:

$$\begin{aligned} m_l \ddot{w}_l &= m_l(-a_0 A\omega^2 \xi_l \cos(\omega t) + \ddot{\epsilon}(t)) \\ &= V'_{l+1}(u_{l+1} - u_l) - V'_l(u_l - u_{l-1}) + V''_{l+1}(u_{l+1} - u_l)(\epsilon_{l+1} - \epsilon_l) \\ &\quad - V''_l(u_l - u_{l-1})(\epsilon_l - \epsilon_{l-1}) + e^* \mathcal{E}(-1)^{l+1}. \end{aligned} \tag{20}$$

To be consistent with the procedure used in the previous section to determine the displacements $u_l(t)$ of the stationary mode, based on the RWA, we have performed a Fourier series of the potential derivatives truncated to first term, obtaining the linearized equations for the perturbation $\epsilon_l(t)$. We have solved these equations numerically, investigating the effects of small perturbations with initial values up to $1/50$ of $u_l(t)$ and initial time step of integrating procedure of the order of 10^{-4} of the period of the mode. We started by considering the

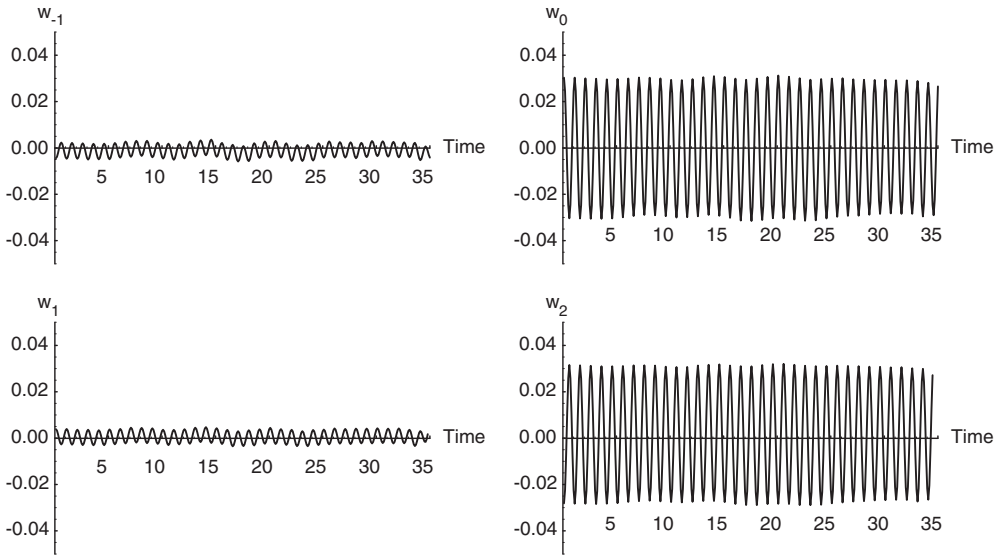

Figure 6. Time evolution of displacement patterns $w_l(t)$ of the ILM mode for $A = 0.03$ without electric field applied. The time is in units of the period $2\pi/\omega$ of the ILM. Only atoms at the centre of the chain are shown.

stationary ILM mode obtained without the electric field. The small perturbations added to the displacement pattern u_l do not grow up during the long time of simulation and the full displacements $w_l(t)$ keep the sinusoidal form of the RWA. In figure 6 are shown the sample results of several tens of periods of simulation for the atoms belonging to the two unit cells at the centre of the chain for $A = 0.03$. Then we have analysed the stability of the combined modes modified by the presence of the electric field of the plasmon. As shown in figure 7 for the case $A = 0.03$ with electric field $\mathcal{E} = 1.6 \times 10^9$ V m^{-1} applied, the effects of the small perturbations are negligible, so we conclude that the combined mode for low amplitude A is stable.

5. Strong anharmonicity

For $A > 0.10$ the potential of equation (1) could not be treated as a harmonic potential in order to apply the theory of the previous section. One has to fully solve equation (1). The intrinsic localized mode without electric field is presented in figure 8 for $A = 0.30$. In this case the localization of the mode involves only a few atoms and the frequency of the mode is inside the gap, well below the bottom of the optical branch. In figure 9 we present the dynamical displacement pattern for $A = 0.30$ and $\omega_p = 500$ cm^{-1} corresponding to an electric field $\mathcal{E} = 1.5 \times 10^8$ V m^{-1}. The frequency of this mixed mode is 536.3 cm^{-1}. The static displacements, not shown in the figure, are different from zero (of the order of 0.10 in the present case) only for the cells close to the origin. Aside from the ILM mode (the region around the atom 'zero') one sees that in each cell there is a uniform polarization. The relative displacement of the atoms in such a unit cell is $|\vec{u}| = |\vec{u}_i^+ - \vec{u}_i^-| = 0.007$. If one considers an infinite chain the averaged polarization of the entire chain is dominated by the positive local polarization so that the dielectric function is positive and the combined mode does not exist. However, for a finite chain, which can represent a thin film or a nanowire [9], the large negative

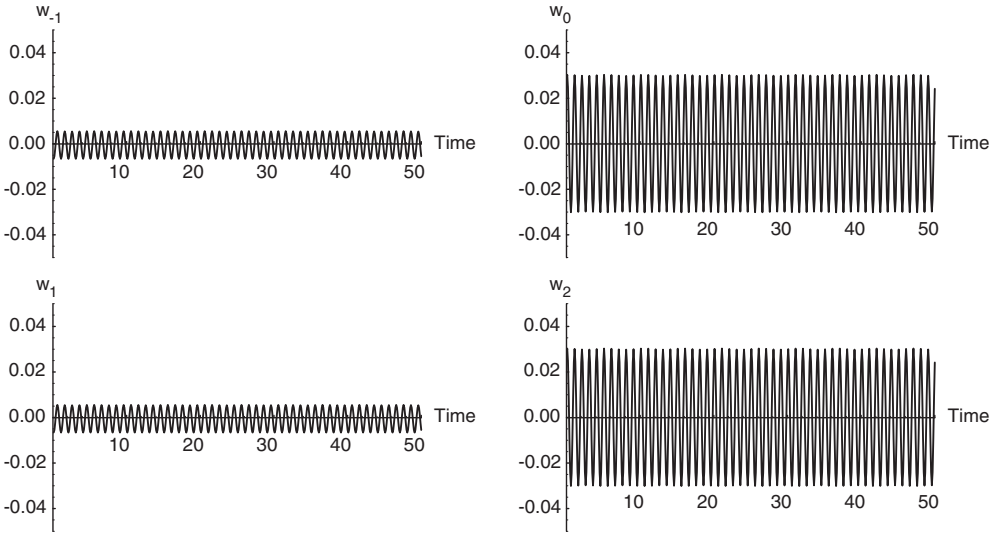

Figure 7. Time evolution of displacement patterns $w_l(t)$ of the combined mode for $A = 0.03$ with electric field $\mathcal{E} = 1.6 \times 10^9$ V m^{-1} applied. The time is in units of the period $2\pi/\omega$ of the mode. Only atoms at the centre of the chain are shown.

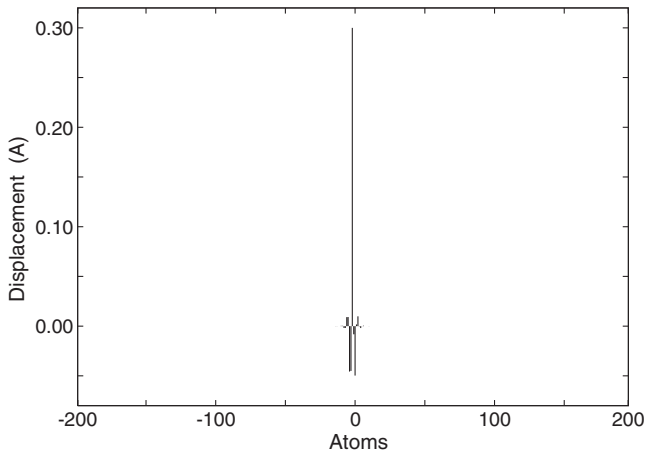

Figure 8. Dynamical displacement patterns of the ILM mode for $A = 0.30$ without electric field applied.

contribution of the ILM to the polarization even if localized over a few cells can balance the positive contribution of the other cells.

We found for example that for amplitude $A = 0.50$, with plasma frequency near the frequency of the ILM obtained for undoped GaN, i.e. in the range $200 \leqslant \omega_p \leqslant 500$ cm^{-1}, and with a number of cells of the order of $N = 100$–300, depending on the electric field of the plasmon, the condition $\epsilon(\omega) = 0$ is verified to within 5% of accuracy. On increasing the amplitude A, the thickness of the slab increases and the number of cells needed to fulfil the condition $\epsilon(\omega) = 0$ increases up to 1000. The stability criterion of section 4 shows that for the high anharmonicity case the combined mode is stable only for a few periods, as shown in figure 10. At the beginning the atoms oscillate around the values of the static displacements, while for larger times the atoms acquire large displacements, making the crystal unstable.

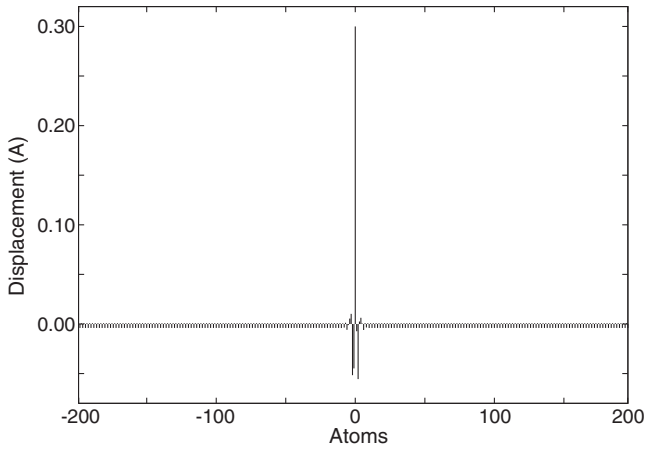

Figure 9. Dynamical displacement patterns of the mixed mode for $A = 0.30$ with electric field $\mathcal{E} = 1.5 \times 10^8$ V m^{-1} applied, corresponding to $\omega_p = 500$ cm^{-1}.

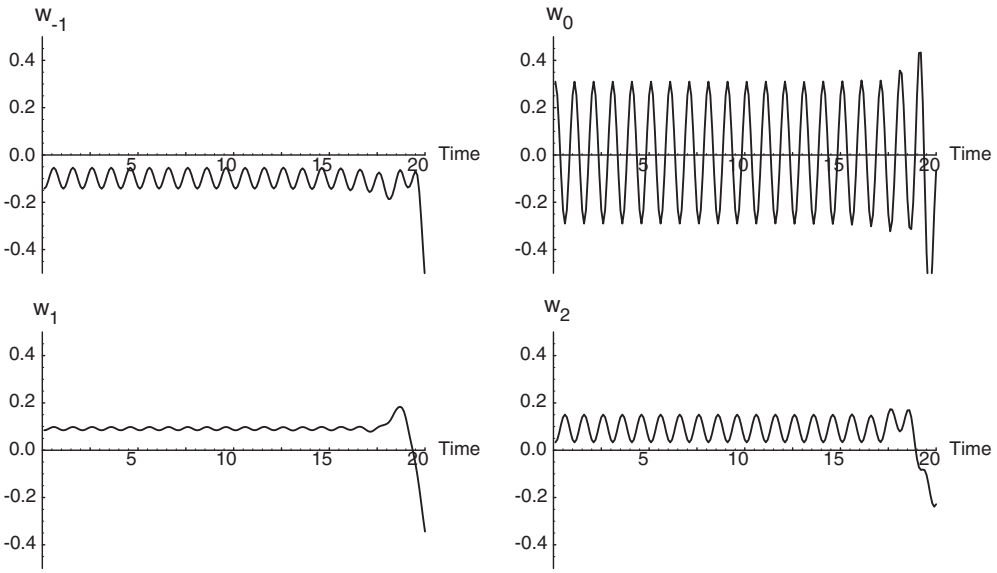

Figure 10. Time evolution of displacement patterns $w_l(t)$ of the combined mode for $A = 0.30$ with electric field $\mathcal{E} = 1.5 \times 10^8$ V m^{-1} applied. The time is in units of the period $2\pi/\omega$ of the mode. Only atoms at the centre of the chain are shown.

In the intermediate region, $0.10 < A < 0.25$, it is not possible to fulfil the condition $\epsilon(\omega) = 0$. One would need a very large electric field, greater than the maximum electric field allowed by the doping range considered, if we analyse the mixed modes above the top of the optical branch, and a too thin slab if we study the mixed modes into the gap.

6. Conclusions

In this paper we have studied the existence of new dynamical vibrational modes generated by the interaction of an ILM and a plasmon. We have considered intrinsic localized modes in a diatomic chain, with alternating masses and interactions. As a test case we took GaN, which has

a large phonon gap. The intrinsic mode lies in the vibrational gap of the semiconductor since we are describing the interaction with a full potential. Donors in the semiconductor produce an electron gas which can oscillate with a frequency both in the gap or above the phonon optical branch, depending on the electron density. In this way we can study the interaction of the ILM with a plasmon with the frequency in a large range of values. We have solved the equations of motion of atoms of the chain numerically in the presence of the electron field associated with the plasmon, and we have studied the dynamical stability of the modes. From the displacement pattern we have derived the polarization of the combined system. The zero of the dielectric function gives the frequency of the combined mode. We have found two main regimes. For small anharmonicity ($A \ll 0.10$) the stable combined mode is above the top of the phonon frequencies. In this case we have shown that the calculated frequency is consistent with the frequency evaluated in the harmonic approximation by considering the dielectric response of polar lattice vibrations. For large amplitude, for an infinite crystal the modes do not fulfil the vanishing of the dielectric response. However, considering a carrier plasma frequency in the gap, the combined mode exists for a finite chain. For large values of A ($A > 0.25$) the combined mode exists for a chain of about 100–300 unit cells or more, depending on the amplitude A and plasma frequency ω_{p}. The finite chain can represent a thin slab in which the forces between planes can be described by a one-dimensional system. In the case of a finite slab, we have not included the surface modes which could change the displacements of a few atoms at the end of the chain. To a first approximation the inclusion of these modes could alter only the thickness of the slab which fulfils the condition for the existence of the combined mode $\epsilon(\omega) = 0$, without altering our general conclusion. In the intermediate region between small and strong anharmonicity, $0.10 < A < 0.25$, it is never possible to fulfil the condition $\epsilon(\omega) = 0$ in the doping range considered.

Acknowledgment

Two of us (AF and VB) gratefully acknowledge partial financial support by MIUR project COFIN2001.

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