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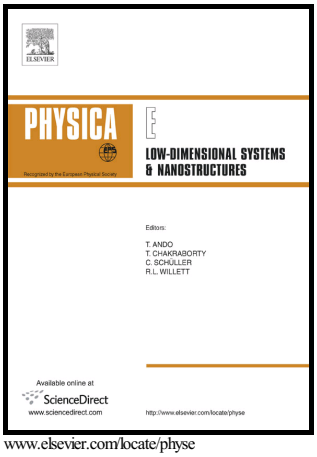

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Dispersion and the Electron-Phonon Interaction in a Single Heterostructure

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Abstract

We investigate the electron-phonon interaction in a polar-polar single heterostructure through the use of the linear combination of hybrid phonon modes, considering the role of longitudinal optical, transverse optical and interface modes, using a continuum model that accounts for both mechanical and electrical continuity over a heterostructure interface. We discuss the use of other models for such systems, such as the bulk phonon (3DP) and dielectric continuum (DC) models, using previously developed sum-rules to explain the limitations on their validity. We find that our linear combination (LC) model gives an excellent agreement with scattering rates previously derived using the 3DP and DC models when the lattice dispersion is weak enough to be ignored, however, when there is a noticeable lattice dispersion, the LC model returns a different answer, suggesting that interface modes play a much greater part in the scattering characteristics of the system under certain conditions. We also discuss the remote phonon effect in polar/polar heterostructures.

Keywords

Semiconductor heterostructures, phonon modes, hybrid model, scattering.

1. Introduction

For many semiconductor nanostructures of engineering interest, the focus of theory is on the interaction of electrons with the polar optical modes of the material, and it is this interaction that is central to the subject of the present paper. The classical treatment of polar optical waves by Born and Huang [1] focuses on electromagnetic dispersion, but ignores lattice dispersion. Most subsequent treatments of the interaction with electrons have also ignored lattice dispersion, since the interaction favours long waves, which are only weakly affected by lattice dispersion. In bulk materials, this is a reasonable assumption to make. However, when investigating nanostructures, the confinement tends to eliminate these long waves and the presence of the interface (IF) modes requires the existence of dispersion. In what follows we demonstrate that this is the case and discuss the limits of validity of other approaches that use simple models to determine the scattering in nanostructures.

There are two aspects to this problem: (1) the nature of the confinement of electrons in structures of nanometre dimensions, and (2) the nature of confinement of the polar optical phonons. In both cases confinement is governed by appropriate connection rules that apply at the boundaries of the

structure. For electrons, the connection rules are the continuity of the wave function and of its gradient. Where the wavefunction is a Bloch function, it turns out that in most cases, the continuity of the gradient of the wavefunction can be replaced by the continuity of $\frac{1}{m^*}\frac{dF(z)}{dz}$, where m* is the effective mass and F(z) is the envelope function, with z along the normal to the boundary [2]. (For conditions under which this replacement may fail, see [3].) For polar modes, the connection rules are the continuity of ionic displacement (**u**) and mechanical stress, together with the standard electromagnetic boundary conditions [4-8]. Satisfaction of these rules determines the allowed eigenstates of the phonons. Such modes in the continuum model take the form of hybrid modes, which are the linear combination (LC) of longitudinally polarized optical (LO) modes, transversely polarized optical (TO) modes, and interface (IF) modes, all necessarily at the same frequency. The resultant waveforms derived in the continuum model are in excellent agreement with those derived numerically in microscopic models of the lattice dynamics [9]. The LC (or hybrid) model, although a continuum model, therefore reliably describes the correct eigenfunctions.

Nevertheless, in most calculations of the electron-phonon interaction, it is common practice to ignore the mechanical connection rules and rely solely on the electromagnetic boundary conditions, regarding the material as simply a dielectric continuum, an approach that dates back to Fuchs and Kliewer's treatment of the polar slab, which introduced electromagnetic interface modes [10]. Subsequently, this dielectric continuum (DC) model has been the model of choice (or the foundation of other models, such as the Huang-Zhu model) in the evaluation of the electron-phonon interaction [11-13]. An even simpler model that has been used frequently is to regard the polar modes as three-dimensional phonons (3DP) [8, 14, 15]. Neither the DC nor the 3DP model use the correct normal modes, but they seek justification in sum-rules that claim that the total electron-phonon scattering rate is independent of the phonon basis set, provided it is complete and orthonormal and satisfies both mechanical and electromagnetic boundary conditions [16, 17]. Register's sum-rule includes the necessity all modes have the same frequency [16]. Mori and Ando made a closely related claim with their sum-rule, stating that all modes should have the same interaction strength [18]. Conversely, the DC model, which takes LO, barrier IF and well IF modes into account, suggests that all these modes are of different frequencies and strength (which is at odds with the premises of these sum-rules), and thus, this justification for use of the sum-rules to validate these models is flawed. While it is interesting to note that the use of this sum-rule can seem valid in many situations, for example, it has been found that a comparison of LC and DC rates for a quantum well support these sum-rules [19], it is extremely important to note there are situations where the use of these sum-rules break down when using these simpler models - a recent comparison of 3DP and DC rates in a single heterojunction shows some departure from these rules [20]. These sum-rules further assume a thermodynamic equilibrium spectrum for the phonons and therefore cannot be expected to hold in cases where there are hot phonons effects or coupling between plasmons and phonons. Such hot phonons and coupled modes are bound to be present in high-power nanostructure devices, further reducing the justification for the use of the sum-rules to validate the models when used for nanostructures. We therefore deduce

that sum-rule predictions have only limited validity and that the LC model can give a more reliable description of the electron-phonon interaction in nanostructures.

In what follows, we present, for the first time (as far as the authors are aware), an application of the LC model to the case of a single heterostructure in which there is a quasi-2D electron gas established in the well at the interface between barrier and well due to barrier polarization. In Section 2, we apply the LC model to a heterostructure, and we note that the polarity of the materials mean that fields are induced in the adjacent layers, allowing the phenomenon of remote-impurity scattering. This in turn excites ionic displacements that have to be considered in establishing the connection rules at the interface. In Section 3 we derive expressions for the scattering rate. We show that the model can be simply interpreted in terms of a LO-like contribution and an IF-like contribution, similar to the DC model. In Section 4 we discuss the role of lattice dispersion and make a comparison with the results obtained by the DC and 3DP models. We then draw conclusions on this work in Section 5. In many practically important cases coupled modes and hot phonons make their appearance, rendering simple models inapplicable. In these cases, the LC model must be used.

Throughout this communication we adopt the simplifying assumption of isotropy and assume dispersion is quadratic in wave vector. We also assume that the crystals that make up the heterostructure are both polar, though we note that the effects of remote-impurity scattering can be eliminated if one of the components of the heterostructure is non-polar.

2. The LC Model

We model our heterostructure as two polar materials, joined at a simple, straight interface. The materials are assumed to be large enough to not cause any confinement effects above those caused by the interface itself. We take the z direction to be normal to the interface between barrier and well situated at z=0; and, exploiting isotropy, we take the x direction to be in the plane of the interface. We define the barrier to be in the region $z \leq 0$, and the well to be in the region $z \geq 0$. This model of the heterostructure is depicted in Figure 1, along with the phonon modes that we consider.

Satisfying the mechanical connection rules in general is not a trivial problem. Unlike the corresponding rules for acoustic modes, the boundary conditions for optical modes involve the spatial variation of ionic mass, a complication first pointed out by Akero and Ando [21] and confirmed in detail using a microscopic model by Foreman and Ridley [7]. Establishing connection rules across the interface between barrier and well involves the consideration of the variation of not only the mass, but also the force constants, the elastic stress and the amplitude of the ionic displacement. Fortunately, in most practical cases, the disparity of the properties between barrier and well are so large that it is reasonable to adopt the simple condition that there is no ionic displacement at the boundary, that is, $\mathbf{u}=0$ at z=0.

In the well ($z \geq 0$), we take the x and z components of the particle displacement to be a linear combination of LO, IF and TO components, observing that the TO displacement has both x and z components:

$$u_x = e^{i(q_x x-\omega t)}\left(q_x A\cos q_z z + q_x B\sin q_z z + q_x Ce^{-q_x z} + \eta De^{-\eta z}\right)$$
$$u_z = ie^{i(q_x x-\omega t)}\left(q_z A\sin q_z z - q_z B\cos q_z z + q_x Ce^{-q_x z} + q_x De^{-\eta z}\right) \quad 1$$

q (its components being q_x & q_z) is the wave vector and all components have the same frequency, that of the LO component. Including the wave vector amplitudes means that the LO components can be seen to satisfy the condition $\nabla \times \boldsymbol{u_{LO}} = 0$, and the IF and TO components satisfy $\nabla \cdot \boldsymbol{u_{IF}} = 0$ (and $\nabla \times \boldsymbol{u_{IF}} = 0$ as a result of adopting the unretarded model). The lattice dispersion, assumed to be quadratic, gives:

$$\omega^2 = \omega_L^2 - \mathrm{v}_L^2(q_x^2 + q_z^2) \quad 2$$

where ω_L is the zone-centre LO frequency and v_L is a velocity (which in the simplest case is the velocity of longitudinal acoustic phonons.)
The TO frequency is similarly described:

$$\omega^2 = \omega_T^2 - \mathrm{v}_T^2(q_x^2 + q_T^2) \quad 3$$

where ω_T is the zone-centre TO frequency and q_T is the TO wave-vector.
Extension to the complex band structure allows the frequency to be equal to the LO frequency, setting $q_T^2 = -\eta^2$ yields:

$$\eta^2 = q_x^2 + \tfrac{1}{v_T^2}\left[\omega_L^2 - \omega_T^2 - v_L^2\left(q_x^2 + q_z^2\right)\right] \quad 4$$

The IF mode is determined by electromagnetic dispersion, $\omega^2 = c^2(q_x^2 + q_{IF}^2)$, where c is the velocity of light and q_{IF} is the wavevector of the interface mode. The latter is comparatively very large, so for the frequency to be equal the LO frequency, $q_{IF}^2 = -q_x^2$.

Associated with these displacements in the well is an electric field:

$$\mathbf{E} = \alpha_0 \frac{1}{\varepsilon(\omega) - \varepsilon_\infty}\mathbf{u} \quad 5$$

where:

$$\alpha_0 = \frac{e^*}{V_0\varepsilon_\infty}, \quad e^{*2} = \omega_T^2 \overline{M} V_0(\varepsilon_s - \varepsilon_\infty) \quad 6$$

e* is the ionic charge, ω_T is the TO frequency, V_0 is the volume of the unit cell, $\varepsilon_{s,\infty}$ are the static and high-frequency permittivities and $\overline{M}$ is the reduced mass of the optical vibration. There is also an induced field in the barrier:

$$E_{Bx} = q_x Fe^{i(q_x x-\omega t)+q_x z}$$
$$E_{Bz} = -iq_x Fe^{i(q_x x-\omega t)+q_x z} \qquad z \le 0 \quad 7$$

The dielectric functions associated with the LO mode (including the effect of dispersion) and the IF mode are:

$$\varepsilon_{LO}(\omega) = \varepsilon_\infty \frac{\omega^2 - \omega_L^2 + \mathrm{v}_L^2(q_x^2 + q_z^2)}{\omega^2 - \omega_T^2 + \mathrm{v}_L^2(q_x^2 + q_z^2)} = 0 \quad 8$$

$$\varepsilon_{IF} = \varepsilon_\infty \frac{\omega^2 - \omega_L^2}{\omega^2 - \omega_T^2} \quad 9$$

The electric displacement for the LO component is **D**=0. The TO component has no electric field.

We choose amplitudes B, C and D to satisfy **u**=0 and the electric field to satisfy the electric boundary conditions. As a result we obtain:

$$u_x = Aq_x e^{i(q_x x-\omega t)}\left(\cos q_z z - \Gamma \sin q_z z - pe^{-q_x z} + [(p-1)/\eta]e^{-\eta z}\right)$$

$$u_z = iAq_z e^{i(q_x x-\omega t)}\left(\sin q_z z + \Gamma \cos q_z z - (q_x/q_z)pe^{-q_x z} + (q_x/q_z)[q_x(p-1)/\eta]e^{-\eta z}\right) \quad 10$$

$$\Gamma = (q_x/q_z)p[1-(q_x/\eta p)(p-1)] \quad 11$$

$$p = [s(1+r)]^{-1}$$

The factors s and r are, respectively, the field factor and the permittivity ratio associated with the IF mode:

$$s = \frac{\omega^2-\omega_T^2}{\omega_L^2-\omega_T^2} \quad 12$$

$$r = \varepsilon_W(\omega)/\varepsilon_B(\omega)$$

The subscripts W and B refer to the property associated with the well and barrier, respectively. The amplitude of the field in the barrier is:

$$F = -\alpha_0 srpA \quad 13$$

We can now exploit the weakness of the lattice dispersion and take $\eta \to \infty$. This effectively removes the effect of the TO mode except for its role in eliminating u_x. With this simplification the scattering potential is given by:

$$\phi = i\alpha_0 Ae^{i(q_x x-\omega t)}\left(\cos q_z z - \Gamma \sin q_z z - spe^{-q_x z}\right) \quad 14$$

$$\Gamma = (q_x/q_z)p$$

Finally, we relate the amplitude to the phonon number operators via energy normalization:

$$A = \frac{1}{Q}\left(\frac{\hbar}{2\bar{M}\omega}\right)^{1/2}(a_{\mathbf{q}} + a_{-\mathbf{q}}^{\dagger}) \quad 15$$

$$Q^2 = \frac{1}{2}(q_x^2+q_z^2)(1+\Gamma^2) + \frac{pq_x(2+p)}{L} \xrightarrow{L\to\infty} \frac{1}{2}(q_x^2+q_z^2)(1+\Gamma^2) \quad 16$$

We have assumed periodic boundary conditions, and, taking L as very large, we have ignored the contribution to the total energy from the induced modes in the barrier.

2.1 Remote-phonon effects

The optical modes in the barrier can be treated similarly. As a result, fields at the barrier frequency are induced in the well whose amplitude is the barrier equivalent of eq. 13:

$$E_{Wx} = -q_x \alpha_{0B} s_B r^{-1} p_B A_B e^{-q_x z}$$

$$E_{Wz} = iq_x \alpha_{0B} s_B r^{-1} p_B A_B e^{-q_x z} \quad 17$$

$$p_B = [s_B(1+r^{-1})]^{-1}$$

The subscript B indicates barrier properties, e.g. frequencies ω_{LB}, ω_{TB} etc. The potential associated with these fields is:

$$\phi_B = -i\alpha_{0B} s_B p_B A_B e^{-q_x z} \quad 18$$

where A_B is the barrier equivalent of A in eq. 15. The effect of this potential on electrons in the well is referred to, somewhat confusingly, as remote-phonon (RP) scattering. Its role in determining the scattering rate in the well is weak, except in the case when r=-1. As well as the scattering, there is another aspect of the RP effect than needs to be considered. In polar materials, fields are related to ionic displacement (eq. 5). This implies that RP fields induce ionic displacements that would seem to violate the condition that **u**=0 at the interface. As shown in Appendix A, the condition **u**=0 is maintained by the induction of a hybrid of evanescent LO and TO modes at the barrier frequency.

It is important to note that RP modes will only occur if the heterostructure is a polar/polar structure. A polar/non-polar structure would eliminate RP scattering in the polar region.

3. Scattering rate

The scattering rate can be written:

$$W = \frac{2\pi}{\mathrm{h}}\frac{1}{N}\sum_{\mathbf{q}}\left|H_{ep}\right|^2\delta(E'-E\pm\mathrm{h}\omega)N(E') \qquad 19$$

The interaction Hamiltonian is:

$$H_{ep} = \int \Psi^*(\mathbf{r})e\phi(\mathbf{r})\Psi(\mathbf{r})\mathbf{dr} \qquad 20$$

A convenient choice of the electron wavefunctions for transitions within the ground state is the Fang-Howard form:

$$\Psi(\mathbf{r}) = \sigma^{1/2}e^{ikx}\psi(z)$$

$$\psi(z) = \left(\frac{b^3}{2}\right)^{1/2} ze^{-bz/2}, \quad z\geq 0, \quad b = \left(\frac{33e^2m^*N_e}{8\varepsilon_s\mathrm{h}^2}\right)^{1/3} \qquad 21$$

Integration over the area of the interface (σ) gives:

$$H_{ep} = \delta_{k'_x,k_x\pm q_x}\int_0^L \psi(z)^2 e\phi(z)dz \qquad 22$$

which defines k'_x in terms of the initial electron wave vector and q_x. It is convenient to express the potential with energy normalisation as follows:

$$\phi(z) = i\alpha_0\left(\frac{\hbar}{2\bar{M}\omega}\right)^{1/2} f(q_x,q_z,z)(a_q + a^{\dagger}_{-q})$$

$$f(q_x,q_z,z) = \frac{1}{Q(q_x,q_z)}\left(\cos q_z z - \Gamma\sin q_z z - spe^{-q_x z}\right) \qquad 23$$

This extracts the dependence on q_z and z. Converting the sum to an integral over q_z and extending the limits to ±∞ enables us to write:

$$G(q_x,q_z,z',z) = \int_{-\infty}^{\infty} f(q_x,q_z,z')f(q_x,q_z,z)dq_z L/2\pi = G_1(q_x)G_2(z',z) \qquad 24$$

The integral over z defines a form factor:

$$F(q_x) = \iint \psi(z')^2\psi(z)^2 G_2(z',z)dz'dz \qquad 25$$

The scattering rate then takes the form:

$$W = W_0\frac{1}{2}\left(\frac{2m^*\omega_L}{\mathrm{h}}\right)^{1/2}\frac{\omega_L}{\omega}\left[n(\omega)+\frac{1}{2}\pm\frac{1}{2}\right]\frac{1}{k}\int G_1(q_x)F(q_x)\frac{dq_x}{\sin\theta(k,q_x)} \qquad 26$$

$$W_0 = \frac{e^2}{4\pi\hbar\varepsilon_p}\left(\frac{2m^*\omega_L}{\hbar}\right)^{1/2} \qquad 27$$

$$\frac{1}{\varepsilon_p} = \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s}$$

m* is the electron effective mass, n is the phonon number, k is the electron wave vector, and θ is the scattering angle. Here, the weak dependence of frequency on wave vector has been ignored, and this allows us to make LO-like and IF-like models, as we will show. In an analytic treatment the lattice dispersion should, of course, be included.

There are two aspects of the LC model that depend on the value of r, the ratio of the permittivities. Being a function of frequency, r varies with the dispersion; for long waves r~0 and the LC is LO-like, but at and near the critical condition r=-1, the LC is IF-like. Clearly, an accurate assessment of the overall rate calls for numerical work, but a useful insight can be obtained from an approximate analytical model that exploits the weakening of the interaction with electrons towards large wave vectors.

For small wave vectors we may put r~0 , p~1 and s~1, essentially ignoring dispersion entirely. The LC is then LO-like and the integration over q_z gives:

$$G(q_x,q_z,z',z) = \frac{L}{2q_x}\left(e^{-q_x|z'-z|} - e^{-q_x|z'+z|}\right) \qquad 28$$

Thus, for the LO-like case:

$$G_1(q_x) = \frac{L}{2q_x}, \quad G_2(z',z) = e^{-q_x|z'-z|} - e^{-q_x|z'+z|} \qquad 29$$

from which the form factor can be calculated. The first term in the expression for G_2 is that obtained for bulk phonons, the second for IF modes. Because the z component of the IF mode displacement is opposed to that of the LO component, the accompanying fields are also opposed, hence the minus sign. Moreover, in the absence of dispersion there is no remote-phonon effect and the IF contribution is simply to counter the effect of the LO mode.

For r~-1, the integration is less straightforward - p–>∞ , and the modes contributed by the barrier become important. This condition occurs at two frequencies $\omega_\pm$, ω_+ being barrier-like, ω_- being well-like, in what follows, the subscripts + and – refer to barrier and well-like properties when this condition (at r~-1) is met.

At both frequencies, the wave vectors at which the condition occurs are typically very large. The conservation of crystal momentum restricts q_x to be typically of order $q_0 = (2m^*\omega/\hbar)^{1/2}$, which is relatively small, in which case q_z is typically very large, say q_{z-} associated with the lower frequency, q_{z+} associated with the upper frequency. The scattering potential is then dominated by the well and barrier IF components, each having the form:

$$f(q_x,q_z,z')\,f(q_x,q_z,z) = \frac{1}{Q^2(q_x,q_z)}s^2p^2e^{-q_x|z'+z|} \approx \frac{2s^2e^{-q_x|z'+z|}}{\left(q_z^2s^2(1+r)^2+q_x^2\right)} \qquad 30$$

We have assumed that $q_z >> q_x$. We can then evaluate the integral over q_z for the well by putting

$$\omega^2 = \omega_-^2 - v_{LW}^2 \Delta q_z^2$$
$$1 + r = -(q_z^2 - q_{zW}^2) r_{\infty -} v_{LW}^2 T_-^2 \qquad 31$$

Similarly, for the barrier mode:

$$\omega^2 = \omega_+^2 - v_{LB}^2 \Delta q_z^2$$
$$1 + r = -(q_z^2 - q_{zB}^2) r_{\infty +} v_{LB}^2 T_+^2 \qquad 32$$

where q_{zW} and q_{zB} are the values of q_z in the well and barrier respectively, corresponding to the condition 1+r=0. We have further defined

$$\mathrm{T}_\pm^2 = \pm \left[\frac{2\omega_\pm^2 - \omega_{LB}^2 - \omega_{TW}^2}{(\omega_\pm^2 - \omega_{LB}^2)(\omega_\pm^2 - \omega_{TW}^2)} - \frac{2\omega_\pm^2 - \omega_{LW}^2 - \omega_{TB}^2}{(\omega_\pm^2 - \omega_{LW}^2)(\omega_\pm^2 - \omega_{TB}^2)} \right] \qquad 33$$
$$r_\infty = \varepsilon_{W\infty} / \varepsilon_{B\infty}$$

For a derivation of $T_\pm^2$, refer to Appendix B. Ignoring the variation in the field factor with q_z, we obtain:

$$G_\pm(q_x, q_z, z' z) = \frac{L}{2q_x} \frac{s_\pm}{r_{\infty\pm} \mathrm{v}_{L\pm}^2 q_{z0\pm}^2 \left|\mathrm{T}_\pm^2\right|} e^{-q_x|z'+z|} = \frac{L}{2q_x} \frac{s_\pm}{r_{\infty\pm}(\omega_{L\pm}^2 - \omega_\pm^2)\left|\mathrm{T}_\pm^2\right|} e^{-q_x|z'+z|} \qquad 34$$

$$r_{\infty +} = r_\infty^{-1},\ r_{\infty -} = r_\infty$$
$$\omega_{L-}^2 = \omega_{LW}^2,\ \omega_{L+}^2 = \omega_{LB}^2$$

Thus, for the IF –like case:

$$G_1(q_x) = \frac{L}{2q_x} \frac{s_\pm}{r_{\infty\pm}(\omega_{L\pm}^2 - \omega_\pm^2)\left|\mathrm{T}_\pm^2\right|}, \quad G_2(z', z) = e^{-q_x|z'+z|} \qquad 35$$

G_1 and G_2 can be used in eq. 26 for the RP barrier rate , where ε_p and the LO frequency are quantities determined by the properties of the barrier.

In summary, we note that the overall scattering rate can be seen approximately to be the sum of three processes:

$$W_{total} = W_{WLO}\big|_{r\approx 0} + W_{WIF}\big|_{1+r\approx 0} + W_{BIF}\big|_{1+r\approx 0} \qquad 36$$

In this respect of this structure the LC model and the DC model are in agreement.

4. Discussion

It is interesting to observe that in the absence of lattice dispersion the hybrid modes are purely LO-like in the meaning of our previous discussion. There are no RP effects, and the role of the IF mode is to *reduce* scattering. To include dispersion is therefore essential in any coherent theory of the electron-phonon interaction in the case of the single heterojunction, or, indeed, any other nanostructure, otherwise that famous condition associated with IF modes, 1+r=0, becomes unachievable without resorting to the complex dispersion branches. The DC model, by its very nature, has no need for dispersion other than that associated with electromagnetic waves, and it can consider the existence of IF modes and their accompanying condition 1+r=0 as a purely electric phenomenon.

We remind the reader of the basic elements of the DC model following Mori and Ando [18]. It chooses two modes that independently obey the

electrical connection rules, but not the mechanical ones. These modes are LO and IF, normalized in the cavity –L <z< L with the interface at z=0. The half-space LO has the potential:

$$\varphi_{LO} = i\alpha_0 A_{LO} 2\sin q_z z$$

$$A_{LO}(q) = \frac{1}{(q_x^2 + q_z^2)}\left(\frac{\hbar}{2\bar{M}\omega_L}\right)^{1/2} \quad 37$$

The IF potential is:

$$\phi_{IF} = i\frac{1}{q_x} A_{IF} e^{i(q_x x - \omega t)} e^{-q_x z}$$

$$A_{IF}(q_x) = \left(\frac{q_x L}{\varepsilon_0 V_0}\frac{1}{\beta_B^{-1} + \beta_W^{-1}}\right)_{\pm}^{1/2}\left(\frac{\hbar\omega_{\pm}}{2}\right)^{1/2}(a_{q_x} + a_{q_x}^{\dagger}) \quad 38$$

$$\beta = \frac{\omega_L^2 s^2}{\omega^2(\varepsilon_p/\varepsilon_0)}$$

As regards scattering rates, the half-space LO mode gives:

$$G(z', z) = \frac{L}{2q_x}\left(e^{-q_x|z'-z|} - e^{-q_x|z'+z|}\right) \quad 39$$

Comparing this with eq. 29, the scattering rate for LO modes as determined by the LC model, we note that the rate is the same. We can also see that it is the same as that for the zero-dispersion model. This should not be a surprising result, recall that when deriving expressions for the LO-like modes, we set parameters that essentially ignored the lattice dispersion.

The IF mode has no dependence on q_z and gives the rate:

$$W = W_0\left(\frac{\omega_{\pm}}{\omega_{WL}}\right)^{1/2}\frac{(\varepsilon_p/\varepsilon_0)_W}{(\beta_B^{-1} + \beta_W^{-1})_{\pm}}\left(\frac{2m^*\omega_{\pm}}{\hbar}\right)^{1/2}\frac{1}{2k}\left((n(\omega_{\pm}) + \frac{1}{2} \pm \frac{1}{2}\right)\int F(q_x)\frac{1}{q_x}dq_x\, d\theta \quad 40$$

Comparing this with eq. 35, we can immediately see that this rate is quite a different result from that predicated by the LC model. This can, at least partially, be attributed to the inclusion of lattice dispersion in the LC model, something that is neglected in DC and 3DP models.

It is clear that there is a close similarity between the two models, but the details are different and the agreement can only be approximate. Nevertheless, where the contribution from the IF mode is weak, (Mori and Ando point out this is frequently the case [18]), the agreement can be close.

We can also see that in the 3DP model, the rate is almost the same as the LC model with zero dispersion, the exception in the rate being:

$$G(z', z) = \frac{L}{2q_x}e^{-q_x|z'-z|} \quad 41$$

Compare this with eqs. 29 and 39. We can see that, in comparison, eq. 41 only contains a"bulk phonon" term, neglecting the IF term entirely. However, as the IF modes contributions tend to be weak in both the LC and DC models, the 3DP model, neglecting this mode altogether, tends to be a reasonable approximation to make.

We can see (from eq. 8) that dispersion does not alter the dielectric function associated with the LO component. We have assumed that the strength

of the interaction with the electron, principally involving long wavelength phonons, is not affected by dispersion. The implication of this is that the effective ionic charge is not a function of wave vector, but this needs to be examined critically.

Whilst we have analysed the scattering in the heterostructure close to thermodynamic equilibrium through the use of the LC model, in high-power devices, the conditions are far from being in such equilibrium. The sum-rules that were used to validate the various simple models assume thermodynamic equilibrium for the phonons, thus, the use of these simple models to describe the electron-phonon interaction in such cases is questionable. The simple models in question include the LO-like and IF-like analysis of the LC model, whose results are encapsulated in eqs. (28-36). In practical systems the electrons become extremely hot and the phonon population is driven far from thermodynamic equilibrium. The hot phonon populations are far from being uniform over frequency, as a consequence of variations in emission rate and phonon lifetime. There are also coupled-mode effects, which are limited to small wave vectors where Landau damping is weak, and cause static screening where Landau damping is strong. While these simple models are limited to the zone-centre LO frequency and the IF frequencies, the relevant phonon numbers are far from equilibrium values, and have to be determined in (ideally) a self-consistent way.

5. Conclusions

We have described a model of polar optical phonons in a single heterostructure in which both mechanical and electrical boundary conditions are satisfied and lattice dispersion is taken into account. This is shown to require a linear combination LO, TO and IF modes. Using an approximation that ignores the contribution of the TO mode everywhere except at the interface between barrier and well, we give expressions for the resultant electron scattering rates. We then describe a model in which the hybrid modes can be approximately analysed as LO-like or IF-like. A comparison is made with the DC model, which ignores mechanical boundary conditions, revealing a similarity of form but differences of detail. We conclude that the DC model can give only an approximate account of the electron-phonon interaction, with agreement getting better when the contribution from the IF modes is weak. A weak contribution from IF modes also supports the use of the bulk phonon approximation. It can be seen that if lattice dispersion is ignored, any positive contribution to the scattering rate from IF modes is eliminated, instead only reducing the scattering rate of the LO mode. Finally, we point out that in practical devices, the description of effects due to coupled plasmon-phonons and to hot phonons require the use of the correct eigenfunctions that the LC model provides.

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Appendix A: Remote-Phonon evanescent modes

Because of lattice dispersion, electric fields at the well frequency appear in the barrier and, equally, electric fields at the barrier frequency appear in the well. These fields are responsible for so-called remote-phonon scattering. Besides their effect on scattering, these remote-phonon fields are associated with corresponding lattice displacements according to eq. (5), which has consequences for the connection rules at the interface. Thus, for example, the fields depicted in eq. (17) will be associated with displacement components u_x and u_z in the well, which are non-zero. This violates the condition **u**=0 at the interface. The condition is restored provided that the IF mode in the well is a component of a hybrid of LO and TO modes, all at the barrier frequency. A corollary of our assumption that **u**=0 at the interface is that there is a large disparity between the frequencies of well and barrier; consequently, the LO and TO components will be heavily evanescent, with exponents derived from the optical-acoustic complex band structure. The barrier hybrid at the well frequency then has the form (z>0):

$$u_x = e^{i(k_x x-\omega t)}\left(k_x P e^{-\eta_L z} + \eta_T Q e^{-\eta_T z} + k_x \mathrm{Re}^{-k_x z}\right)$$
$$u_z = ie^{i(k_x x-\omega t)}\left(-\eta_L P e^{-\eta_L z} + k_x Q e^{-\eta_T z} + k_x \mathrm{Re}^{-k_x z}\right) \quad \text{A.1}$$

Solving for u_x=0 and u_z=0 leads to:

$$u_x = k_x \mathrm{Re}^{i(k_x x-\omega t)}\left(-p_L \frac{1-p_T}{1-p_L p_T} e^{-\eta_L z} - \frac{1-p_L}{1-p_L p_T} e^{-\eta_T z} + e^{-k_x z}\right)$$
$$u_x = ik_x \mathrm{Re}^{i(k_x x-\omega t)}\left(-\frac{1-p_T}{1-p_L p_T} e^{-\eta_L z} - p_T \frac{1-p_L}{1-p_L p_T} e^{-\eta_T z} + e^{-k_x z}\right) \quad \text{A.2}$$

In these equations:

$$p_L = \frac{k_x}{\eta_L}, \quad p_T = \frac{k_x}{\eta_T} \quad \text{A.3}$$

As regards the effect on the electrical connection rules, the TO component has no effect, while the large magnitude of η_L make the contribution to the tangential field negligible. The particle amplitude R can be obtained from the electric fields depicted in eq.(17), which are unchanged.

Appendix B: Derivation of T

What follows is a derivation of T_-, but the steps can equally be applied to the derivation of T_+. We start with the definition from eqns. (8), (12) and (31) to define 1+r, and defining ω_- as the low frequency solution of 1+r=0:

$$1+r = 1+r_\infty \frac{(\omega^2-\omega_{LW}^2)(\omega^2-\omega_{TB}^2)}{(\omega^2-\omega_{TW}^2)(\omega^2-\omega_{LB}^2)}$$
$$= 1+r_\infty \frac{(\omega_-^2-\mathrm{v}_{LW}^2\Delta q_W^2-\omega_{LW}^2)(\omega_-^2-\mathrm{v}_{LW}^2\Delta q_W^2-\omega_{TB}^2)}{(\omega_-^2-\mathrm{v}_{LW}^2\Delta q_W^2-\omega_{TW}^2)(\omega_-^2-\mathrm{v}_{LW}^2\Delta q_W^2-\omega_{LB}^2)} \quad \text{B.1}$$

Performing an expansion of these brackets, and discarding higher order terms (O(4) and above), we obtain

$$1+r = 1+r_\infty \frac{(\omega_-^2-\omega_{LW}^2)(\omega_-^2-\omega_{TB}^2)-\mathrm{v}_{LW}^2\Delta q_W^2(2\omega_-^2-\omega_{LW}^2-\omega_{TB}^2)}{(\omega_-^2-\omega_{TW}^2)(\omega_-^2-\omega_{LB}^2)-\mathrm{v}_{LW}^2\Delta q_W^2(2\omega_-^2-\omega_{LB}^2-\omega_{TW}^2)}$$

$$= 1+r_\infty \frac{(\omega_-^2-\omega_{LW}^2)(\omega_-^2-\omega_{TB}^2)\left[1-\dfrac{\mathrm{v}_{LW}^2\Delta q_W^2(2\omega_-^2-\omega_{LW}^2-\omega_{TB}^2)}{(\omega_-^2-\omega_{LW}^2)(\omega_-^2-\omega_{TB}^2)}\right]}{(\omega_-^2-\omega_{TW}^2)(\omega_-^2-\omega_{LB}^2)\left[1-\dfrac{\mathrm{v}_{LW}^2\Delta q_W^2(2\omega_-^2-\omega_{LB}^2-\omega_{TW}^2)}{(\omega_-^2-\omega_{TW}^2)(\omega_-^2-\omega_{LB}^2)}\right]} \qquad \text{B.2}$$

Noting that the Taylor Series expansion of $\frac{1}{1-\alpha} = 1+\alpha-\alpha^2+\alpha^3$, we take the first two terms and subsequently collect like terms to obtain:

$$1+r = 1+r_\infty \frac{(\omega_-^2-\omega_{LW}^2)(\omega_-^2-\omega_{TB}^2)}{(\omega_-^2-\omega_{TW}^2)(\omega_-^2-\omega_{LB}^2)} \times$$

$$\left[1-\frac{\mathrm{v}_{LW}^2\Delta q_W^2(2\omega_-^2-\omega_{LW}^2-\omega_{TB}^2)}{(\omega_-^2-\omega_{LW}^2)(\omega_-^2-\omega_{TB}^2)}\right]\left[1+\frac{\mathrm{v}_{LW}^2\Delta q_W^2(2\omega_-^2-\omega_{LB}^2-\omega_{TW}^2)}{(\omega_-^2-\omega_{TW}^2)(\omega_-^2-\omega_{LB}^2)}\right] \qquad \text{B.3}$$

$$= 1+r_\infty \frac{(\omega_-^2-\omega_{LW}^2)(\omega_-^2-\omega_{TB}^2)}{(\omega_-^2-\omega_{TW}^2)(\omega_-^2-\omega_{LB}^2)}\left[1-\mathrm{v}_{LW}^2\Delta q_W^2 T_-\right]$$

$$T_- = \frac{2\omega_-^2-\omega_{TB}^2-\omega_{LW}^2}{(\omega_-^2-\omega_{TB}^2)(\omega_-^2-\omega_{LW}^2)} - \frac{2\omega_-^2-\omega_{TW}^2-\omega_{LB}^2}{(\omega_-^2-\omega_{TW}^2)(\omega_-^2-\omega_{LB}^2)} \qquad \text{B.4}$$

From our previous definition of ω_-, $r_\infty \frac{(\omega_-^2-\omega_{LW}^2)(\omega_-^2-\omega_{TB}^2)}{(\omega_-^2-\omega_{TW}^2)(\omega_-^2-\omega_{LB}^2)} = -1$, we thus find,

$$1+r = \mathrm{v}_{LW}^2\Delta q_W^2 T_- \qquad \text{B.5}$$

where $\Delta q_W^2 = (q_z^2-q_{z0}^2)_W$

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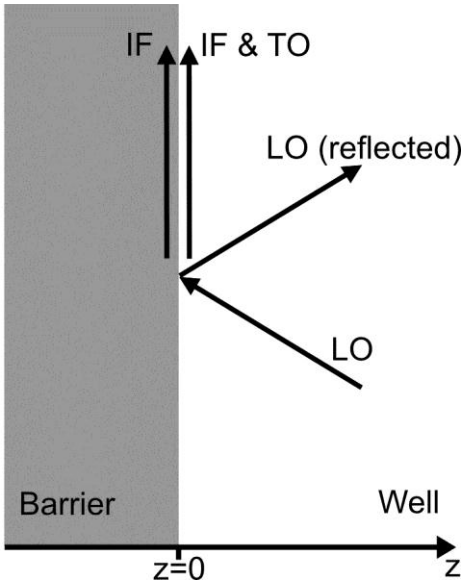

Figure 1: The polar-optical phonon modes generated by an LO mode striking the interface between the barrier and well. LO modes are reflected from the interface back into the well, and IF and TO modes are generated which are evanescent, propagating along the interface. TO modes only exist in the well, IF modes exist on both sides of the interface.

Highlights

- We use the Linear Chain (LC) model for phonons in a single heterostructure.
- Excellent agreement with other models when neglecting dispersion.
- Effects of lattice dispersion can be included and studied using the LC model.
- Inclusion of dispersion suggests interface modes can have an important role.