Transport properties of holes in InP nanowires were calculated considering electron-phonon interaction via deformation potentials, the effect of temperature and strain fields. Using molecular dynamics, we simulate nanowire structures, LO-phonon energy renormalization and lifetime. The valence band ground state changes between light- and heavy-hole character, as the strain fields and the nanowire size are changed. Drastic changes in the mobility arise with the onset of resonance between the LO-phonons and the separation between valence subbands.

Semiconductor nanowires (NWs) are increasingly used in a wide range of devices. They appear as building blocks of nanocircuits and can be applied in electrically driven lasing, which can be used in telecommunications and information storage for medical diagnostics and therapeutics. Improvements in NW synthesis, including chemical technics, allow thorough control of their shape, size and composition along with detailed microscopic characterization of built-in strain fields. As the conductivity is mostly defined by the carrier-phonon interaction and phonon-lifetime, tuning of the NW structural properties could result in the possibility of also finding optimal conditions for carrier transport.

Considerable efforts have been devoted to the description of carriers in the conduction band of NWs, while similar endeavors are not so common for holes in the valence band. As the mobility is inversely proportional to the carrier effective mass, one may naturally expect that considering carriers in the valence band may result in a drop in mobility when compared to the light electrons in the conduction band. This could certainly be the case for heavy-hole (hh) transport; however, light-holes (lh) under certain conditions may be promoted to be the top valence band by tuning structural parameters of NWs. This atypical circumstance is the result of confinement effects and lh-hh mixing, affected as well by strain and surface asymmetry fields. As we will show here, this results in significant mobility enhancement for lh in suitable NWs. We can also take advantage of valence band mass anisotropy to attain resonant conditions that allow sharp variations of the hole mobility with external parameters, especially when the leading scattering process involve longitudinal optical phonons (LO-phonons) through the deformation potential. Additional hole-phonon interactions, such as deformation potential and piezoelectric coupling to acoustic phonons and polar coupling to optical phonons, have weaker effects and will not be considered here. In order to provide realistic estimates of the expected mobility changes in the NWs of interest, we consider the effects of dimensionality reduction on the LO-phonon dispersion and lifetime, using molecular dynamics simulations for different NWs size and at various temperatures.

We consider different NW cross sections and shapes, while temperature effects are included in the mobility through the phonon occupation and strain effects in a multiband Luttinger Hamiltonian. We find that mobility changes in a non-monotonic fashion according to NW width, strain fields, and temperature. In particular, we show that for certain NW widths, one finds resonant behavior that greatly suppresses the hole mobility and is strongly affected by temperature and strain. The interaction potentials used in our molecular dynamics (MD) simulations consist of two- and three-body interaction terms, as described by Branicio et al. The parameters of the interatomic potential are determined using the cohesive energy, density, bulk modulus and elastic constant $C_{11}$ of the material as described before, with some slight adjustments.

This potential provides excellent estimates for melting temperature, structural phase transformation induced by pressure, and specific heat and describes well the vibrational density of states of the material. We obtain the phonon density of states in InP NWs considering different temperatures. The NWs were created cutting a block of a perfect crystal with the $z$-axis along the [001] direction with periodic boundary conditions in the $z$-direction. The $x$- and $y$-directions were surrounded by a vacuum region. The system consisted typically of nine unit cells along $x$- and $y$-directions and forty unit cells along the $z$-direction (53A×53A×234.5A); the total number of atoms is 25,920 (12,960 In + 12,960 P) (Fig. 1(d)). The NW is allowed to relax during a long simulation run (25,000 time steps, one time step=1.5fs) at each temperature. After this relaxation time, a few surface defects can be observed.
Fig. 1. VDOS for NW and bulk. (a) Total VDOS: rigid ion model (RIM) VDOS for bulk from data.\textsuperscript{30} (b) and (c) Partial VDOS for bulk and NW at 300K; (b) indium contribution and (c) phosphorus contribution. (e) and (f) VDOS for bulk and NW at 10 K and 300 K. (d) Simulated InP NW structure by molecular dynamics at \( T = 300K \). Green (grey) dots represent Indium (Phosphorus) atoms.\textsuperscript{51,52}

The effect of the surfaces on the VDOS of the NW is also shown in Fig. 1(a)-(c). The main NW characteristics in the VDOS resemble the bulk results; however, some differences can be observed. The NW surfaces appreciably increases the amount of modes in the gap region, between 22\,meV and 36\,meV (acoustic modes below 22\,meV not shown).

The hole wave function in the NW has the form\textsuperscript{33}:

\[
|\psi_{hh}\rangle = \frac{1}{\sqrt{2}}(|\psi_{\text{lh}}\rangle \pm i|\psi_{\text{hh}}\rangle),
\]

where \( |\psi_{\text{lh}}\rangle \) is the envelope function, which depends on the cross section of the NW, and \( |\psi_{\text{hh}}\rangle \) is the total angular momentum eigenstate, \( |3/2, \pm 3/2\rangle \) for pure hh character, and \( |3/2, \pm 1/2\rangle \) for the lh.

The hole-phonon interaction Hamiltonian is given by

\[
H_{hh} = -\left(\frac{\gamma_1 + \gamma_2}{2}\right)\{\hat{k}_x, \hat{k}_-\} - \left(\frac{\gamma_1 - 2\gamma_2}{2}\right)\hat{k}_z^2,
\]

for the heavy- and light-holes, where \( \gamma_\alpha (\alpha = 1, 2, 3) \) are the Luttinger parameters, \( \{A, B\} = \frac{1}{2}(AB + BA) \), and \( \hat{k}_\pm = \hat{k}_x \pm i\hat{k}_y \). Notice that the subband with hh character along the wire has a low effective mass in the transverse direction \( \approx (\gamma_1 + \gamma_2)^{-1} \), while the lh subband has a large transverse mass \( \approx (\gamma_1 - \gamma_2)^{-1} \); the different transverse masses result in the possible inversion of the lh and hh subband ordering, due to the NW confinement effects. Strain effects lead to modulation of the valence subbands,\textsuperscript{5} introducing a subband displacement given by\textsuperscript{32}:

\[
\Delta H_{hh} = -P + Q \quad \text{and} \quad \Delta H_{lh} = -P + Q + \frac{2\Omega^2}{\gamma},
\]

where \( P = 2(a_v + a_c)(\alpha c^{\gamma}_{11} - \alpha c^{\gamma}_{11})\epsilon_\parallel \), \( Q = -b(c^{\gamma}_{11} + c^{\gamma}_{11})\epsilon_\parallel \), and \( \Delta_\text{SO} = 0.108eV \) is the spin-orbit split-off energy.\textsuperscript{33}

The hole wave function in the NW has the form \( |\Psi_z\rangle = |\psi_{\mp}\rangle |J, m_j\rangle \), where \( |\psi_{\mp}\rangle \) is the envelope function, which depends on the cross section of the NW, and \( |J, m_j\rangle \) is the total angular momentum eigenstate, \( |3/2, \pm 3/2\rangle \) for pure hh character, and \( |3/2, \pm 1/2\rangle \) for the lh.

The mobility is given by \( \mu = \frac{e}{m_0\lambda_{2D} \tau} \), in terms of the hole-phonon scattering time, \( \tau^{-1} = \sum_q S(k, q) \), and the
transition rate

\[
S(k, k') = \frac{2\pi}{\hbar} \left[ |\langle H_{h\rightarrow p}^{\gamma} \rangle|^2 \delta(E_1(k') - E_1(k) - \hbar \omega_{\gamma}) + |\langle H_{h\rightarrow p}^{\gamma} \rangle|^2 \delta(E_2(k') - E_2(k) + \hbar \omega_{\gamma}) \right]
\]

where \( k \) and \( k' \) refers to the initial and final states, and \( H_{h\rightarrow p}^{\gamma} \) and \( H_{h\rightarrow p}^{\gamma} \) refer to the phonon absorption and emission processes in Eq. (4). The phonon density is assumed to be given by a Lorentzian centered at \( \omega_{LO} \) with width \( \gamma \). Both of these values shift with temperature, as discussed in the previous section. We now may analyze the effects of strain and temperature on the hole mobility.

![Fig. 2](image)

**FIG. 2.** Valence band ground states for NW of width \( W \). (a) When the lh occupies the ground state. (b) When the hh occupies the ground state.

To characterize the initial and final states involved in the scattering processes that affect the mobility, we show in Fig. 2 the relevant valence band structure for two different cases. For thin NWs, with or without strain, the finite NW width leads to a picture similar to Fig. 2(a), where the lh subband is promoted to the top given its higher transverse effective mass, as discussed before. Thus, under such conditions, a hh can be scattered to the subband with hh character through phonon emission (process \( A_1 \)), and at \( T > 0 \) the lh can be excited to the hh subband via phonon absorption (process \( A_2 \)). In the presence of lateral compressive strain, the subbands may switch their relative positions with the hh assuming the top at large NW width. Then, a lh might be scattered via phonon emission (process \( A_2 \)) while a hh can be affected by phonon absorption at \( T > 0 \) (process \( A_2 \)). Notice that by changing the wire radius, one can reach a resonant condition (\( \Delta E_{vb} = \hbar \omega_{LO} \)). On the other hand, with strain, depending on the value of the NW width, the ground state can have a character lh (thin NW) or hh (thick). This behavior is similar for all NW cross sections, as it reflect the transversal quantization.

The relative position of the valence subbands is extremely important for the carrier transport in NWs. Given the mobility dependence on the longitudinal effective mass, which modulates the hole-phonon interaction, valence subband shifts may produce sharp fluctuations of the mobility as temperature or structural parameters change. Fig. 3 shows the mobility for different strain and temperature values as function of the NW width. In Figs. 3(a)-(b), the mobility reflects a band configuration similar to the one depicted in Fig. 2(a). At \( T = 70K \), in Fig. 3(a), the increase effect of phonon absorption leads to the monotonic decrease of the lh mobility whit increasing NW width, while the hh displays a monotonic mobility increase, as the intersubband separation decreases with increasing NW width. Also, a sharp variation near the region where \( \Delta E_{vb} \sim \hbar \omega_{LO} \) is seen, the resonant condition greatly enhances LO phonon emission by a hh in panel (a). At higher temperatures, Fig. 3(b), the resonant condition also affects the carriers in the lh subband, producing a sharp drop in mobility (from \( A_1 \) processes).

Given the band structure modulation with strain, the condition \( |\Delta E_{vb}| \sim \hbar \omega_{LO} \) can be attained twice by varying the NW width (corresponding to the cases displayed in Figs. 2(a) and (b)). Thus, two resonant regions appear in Fig. 3(c) where phonons can be emitted by both the lh and hh subbands (\( E_1 \) an \( E_2 \) processes, respectively). At higher temperatures, the phonon absorption features appear as additional jumps in the mobility, shown in Fig. 3(d), processes \( A_1 \) and \( A_2 \). Notice that the lh and hh subband inversion with increasing NW width, in the presence of strain, is accompanied by crossing of the mobility curves, Figs. 3(c)-(d). Tuning the mobility of a hole system via in-situ changes of the NW width or strain fields, is not an easy task in experiments. As we will see below, however, one can achieve drastic in-situ mobility changes for NWs close to the resonance condition by suitable changes in temperature.

![Fig. 3](image)

**FIG. 3.** Hole mobility versus NW width \( W \) for states with \( k_z = 0 \). (a) System at \( T = 70K \) without strain. (b) System at \( T = 300K \) without strain. (c) System at \( T = 70K \) with strain. (d) System at \( T = 300K \) with strain.
and (b) as function of temperature for states with \( k_z = 0 \), (a) as function of strain for \( T = 70K \), and (b) as function of temperature for \( \epsilon_{||} = 0.9\% \). (c) Light hole mobility ratio, where \( \Delta \mu_{lh} = (\mu_{lh}(70K) - \mu_{lh}(300K)) \), versus wire width for different values of strain at \( k_z = 0 \).

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