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E_1 Gap of Wurtzite InAs Single Nanowires Measured by Means of Resonant Raman Spectroscopy

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Abstract. Indium arsenide nanowires were synthesized with an intermixing of wurtzite and zincblende structure by chemical beam epitaxy with the vapor-liquid-solid mechanism. Resonant Raman spectroscopy of the transverse optical phonon mode at 215 cm^{-1} reveals an E_1 gap of 2.47 eV which is assigned to the electronic band gap at the A point in the indium arsenide wurtzite phase.

Keywords: InAs, nanowire, wurtzite structure, Raman spectroscopy, E_1 gap
PACS: 78.67.Uh

INTRODUCTION

Semiconductor nanowires (NWs) have attracted a tremendous amount of interest in recent years and are expected to be critical components in future electronic and optoelectronic devices. InAs with its narrow band gap and its high electronic mobility is particularly convenient for high-frequency electronic applications [1, 2]. Among the several unique properties of semiconductor NWs one can highlight their epitaxial growth in a structural phase that is not available for its bulk counterpart. In the case of InAs NWs, one can achieve either wurtzite (WZ) or zinc Blende (ZB) structures by tuning various growth parameters such as the temperature, the flux ratio of the precursors or the substrate [3].

In this work, we have investigated single InAs NWs grown by chemical beam epitaxy by means of resonant Raman spectroscopy. We have determined the electronic band gap near the A point of the WZ structure and observed that the polarization dependence of the TO vibration in the WZ structure follows the Raman selection rules for the A_1(TO) mode.

EXPERIMENTAL

The NWs were grown by the vapor-liquid-solid method in a chemical beam epitaxy system using gold nanoparticles as catalysts. For the analysis the sample was grown at 480 °C. Transmission electron microscopy (TEM) results show that these NWs contain an intermixing of WZ and ZB structure. The NWs which exhibit a rod-like shape are grown along the [0001] and [111] direction, respectively, and have a diameter of approximately 50 - 200 nm, whereas their length ranges from 5 to 15 μm.

Raman spectroscopy was realized in the backscattering configuration on single InAs NWs transferred onto an Al-covered GaAs substrate. Different lines of a Kr-Ar laser were used for excitation. The scattered light was collected by a triple spectrometer with a charge couple device detector. The laser spot on the sample was about $1-2\,\mu$m.

RESULTS AND DISCUSSION

The inset of Fig. 1a shows a typical Raman spectra where two main vibration modes, similar to the TO and LO mode of the InAs ZB structure, can be identified. For the low energy mode A_1(TO) at $\sim$215 cm^{-1} we observed a resonant Raman scattering for the excitation energy of $\sim$2.47 eV (see Fig. 1a, upper spectrum) in the $x(y,y)\bar{x}$ configuration (using Porto's notation) where z (parallel to [0001]) is the growth direction of the NWs. The resonance is assigned to the E_1 gap of the InAs NW. This value is slightly smaller than the E_1 transition energy of 2.57 eV (dashed line) for ZB InAs measured by Raman spectroscopy (Fig. 1b). Note that the E_1 gap measured by Raman spectroscopy is shifted to higher energies with respect to the E_1 transition obtained by reflectance or absorption spectra [4, 5].

Performed ab-initio calculations of the band structure in WZ and ZB InAs show that the band gap at the A point in the WZ structure (Fig. 2a) is approximately 160 meV smaller than the E_1 gap near the L point in the ZB structure (Fig. 2b). The calculated red-shift of the E_1 gap is consistent with the data obtained experimentally. The slightly smaller red-shift observed in the experiment can

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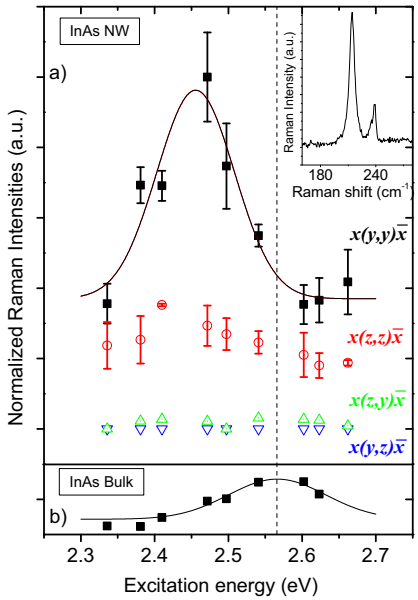

FIGURE 1. Integrated Raman intensities as a function of the laser excitation energy of a single InAs NW for four different polarization configurations (a) and of ZB InAs bulk material (b). The dashed line depicts the E_1 energy transition at the L point of the ZB structure. The solid curves are fitted Gaussians and the error bars represent the standard deviation of the Raman intensities of at least three different spectra taken at the same spot on the single NW. The inset shows a typical Raman spectrum which exhibits two main optical phonon modes.

be associated with the presence of the ZB phase in the structure. Note that the absolute values of the energy gaps do not correspond with the real values, a feature that is often observed in ab-initio calculations. Confinement or strain effects can be neglected due to the large diameters of the NWs (> 50 nm).

In addition, polarization dependent measurements show a much larger Raman cross section for the parallel scattering configurations $x(y,y)\bar{x}$ and $x(z,z)\bar{x}$ configuration than for crossed scattering configurations $x(z,y)\bar{x}$ and $x(y,z)\bar{x}$ (Fig. 1a). This is consistent with the selection rules for the A_1(TO) mode in the WZ structure which is allowed only in parallel scattering configurations [6]. Note that in the parallel configuration, where the incident and scattered polarization is perpendicular to the wire axis, the maximum intensity for the A_1(TO) phonon mode is observed.

We have investigated the electronic E_1 transition of the WZ and ZB phase by means of resonant Raman spectroscopy. The energy of the E_1 gap of the NW was determined at 2.47 eV, slightly smaller than for the ZB InAs bulk material. The shift of the E_1 gap is a consequence of

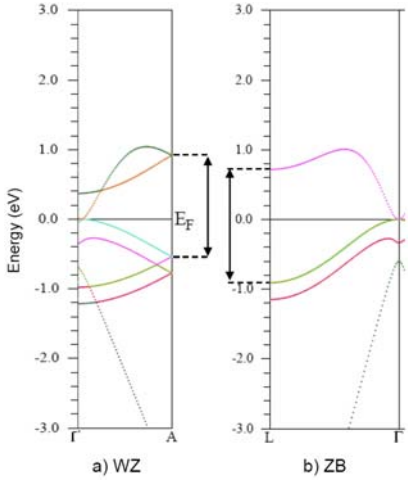

FIGURE 2. Ab-initio calculation of the band structure in WZ (a) and ZB (b) InAs. The key region of interest is where the L point of the ZB structure and the A point of the WZ structure are shown. The arrows denote the gaps between valence and conduction band for the WZ and ZB phase at these symmetry points, respectively.

the WZ phase in the NWs which is supported by an ab-initio calculation of the electronic band structure (Fig. 2).

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