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Progress in Physics (45)

Uniaxial Stress in GaAs Nanowires Reveals an Unprecedented Light Emission Tunability and Novel Bandstructure Transitions

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Uniaxial Stress in GaAs Nanowires Reveals an Unprecedented Light Emission Tunability and Novel Bandstructure Transitions

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The semiconductor industry faces today two of the biggest challenges in its history, i.e. the future of CMOS scaling and the limits in bandwidth and energy of the current technology of interconnects. As the transistor device dimensions (i.e. the technology node) shrink below 100 nm, physical phenomena like size quantization and short channel effects start to interfere with traditional scaling laws. At the same time, the power dissipated in electrical interconnects to enable the communication between an increasing amount of transistors is rising above 80% of the total energy used on the chip, and the amount of heat that can be removed from each chip is saturating [1]. To overcome the limitations in transistor performance and to enable integrated photonic communication on chip, a combination of different strategies has been proposed at the device level: strain engineering, novel materials and device structures.

The nanowire structure has the ideal geometry for the electrostatics of CMOS transistors and, at the same time, allows a direct integration of III-V materials on silicon, enabling ultimate transistor performance and the integration of light sources directly on silicon. Strain engineering would enable the realization of transistors with increased channel mobility and, in the context of active photonic devices, permit to tune the wavelength of emission and improve the performance of solid state lasers (reducing the threshold current, suppressing the Auger recombination and inter valence band absorption processes, controlling the polarization [1]). Inspired by such a wide range of possible applications, we have explored the synergistic interplay of strain effects in III-V nanowires. Nanowires promise exceptional mechanics and a large range of elastic deformation, which can have unexpected effects on their electronic and optical properties.

We apply uniaxial stress to single nanowires exploiting the mechanical degrees of freedom that the substrate can offer (Figure 1). Continuum mechanics teaches us that perfectly uniaxial stress and reproducible mechanical deformations can be obtained and controlled with sub-nanometer resolution by bending a thick substrate on the millimeter scale. In this way, it was possible to apply uniaxial stress mechanically to the nanowire in a continuous and reversible way, both in compression and tension. To investigate the effects of strain on the nanowires we rely on optical spectroscopy: we can obtain an accurate picture of the bandstructure using photo-

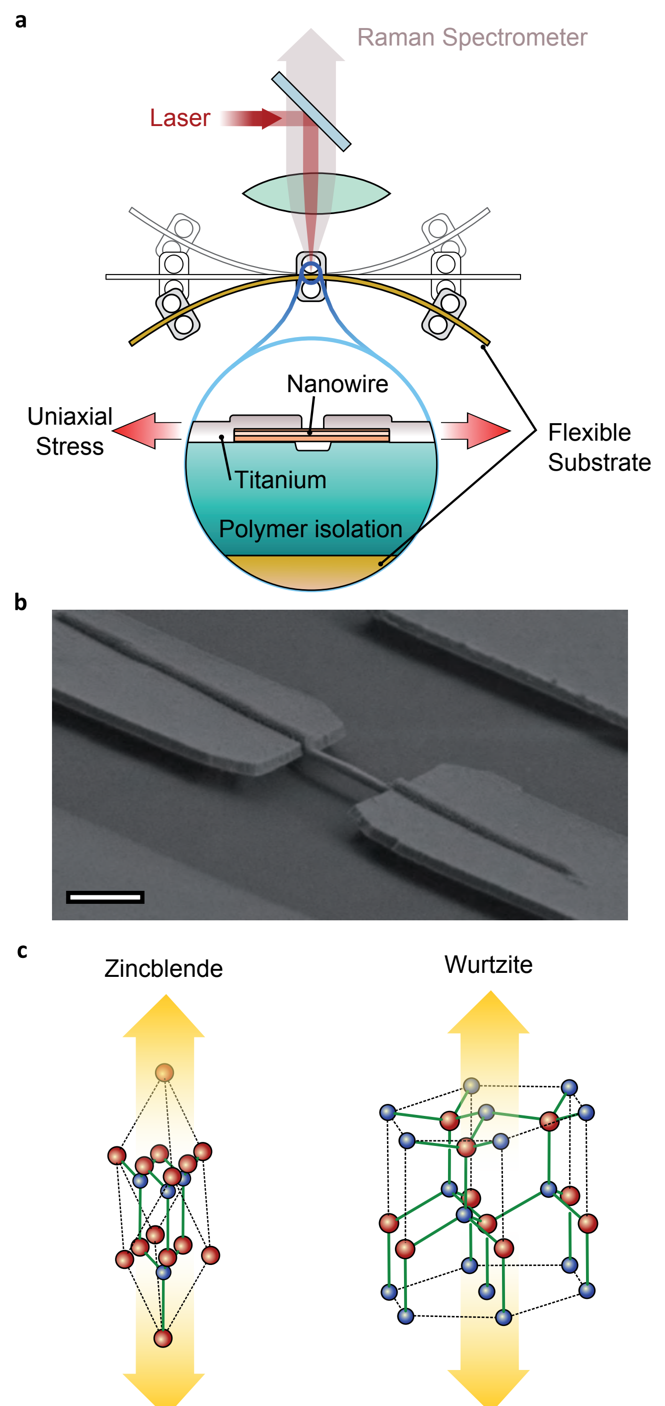

Figure 1. Application of stress to individual nanowires. (a) Schematics of the bending mechanism used to apply stress to individual nanowires structures (shown in cross section). The nanowire is excited using a He-Ne laser, and the PL and Raman signal are collected via an optical spectrometer. (b) Scanning electron microscopy image of a freestanding nanowire clamped by Ti contacts to a flexible substrate. Scale bar is 1 µm. (c) Deformation upon uniaxial stress of the Zincblende (left) and Wurtzite (right) crystal unit cells.

luminescence (PL) spectroscopy, as well as of the lattice dynamics using Raman spectroscopy. Studying such spectra as a function of the polarization can offer a broad insight on the physics of the strain effects. Polarization-dependent PL enables to resolve the symmetry of the conduction and valence band states involved in the light emission processes. In Raman spectroscopy, controlling the polarization of the laser and of the detected light allows the identification of the contribution of individual phonon symmetries. This information can be translated into an estimate of the axial strain and Poisson ratio of the nanowire, which provides together the full characterization of the strain tensor experienced by the nanowire. GaAs was chosen as the ideal material system to study, for many reasons: Zincblende GaAs is considered as the material that enabled the foundations of semiconductor-based solid state lasers and light-emitting devices; when grown at nanoscale dimensions, novel crystal structures like Wurtzite can be synthesized and new degrees of freedom to tailor electronic and optoelectonic properties are available.

Our experiments have shown that, indeed, the nanowire geometry enables the expected enhancement of the strain effects in GaAs. We demonstrated that by tuning the strain continuously, from tension to compression and up to 3.5 %, the PL of Zincblende GaAs nanowires can be red-shifted by 290 meV [2]. We have observed a much more pronounced PL shift in tension than in compression (see Figure 1a), and have attributed this phenomenon to the different symmetry character of the top valence band: heavy hole under tension, light hole under compression. Fingerprints of symmetry breaking due to the anisotropic nature of the nanowire deformation were found also in the Raman spectra, in which polarization-dependent measurements allowed the unambiguous identification of distinct phonon contributions. Because of the linear relation with stress, the energy shift of the Raman peaks (see Figure 1a) were used to determine the axial strain induced in the nanowire and to infer information about the Poisson ratio in the [111] direction (0.16 ± 0.04). To test the consistency of the 8-band k·p model (see Figure 1b) with the measurement, we extracted the band-edge deformation potentials (a = –8.6 eV ± 0.7 eV and d = –5.2 eV ± 0.7 eV), which are consistent with those of bulk GaAs and with our initial assumptions.

Even larger shifts of the PL could be demonstrated by applying strain to Wurtzite nanowires [3]. Using PL spectroscopy and varying the strain over a range of ±2 %, we demonstrated a remarkable energy shift of 345 meV due to transitions between the bright conduction band and the heavy hole band (low energy peak in Figure 3a), and a smaller shift of 257 meV for transitions involving the light hole band the bright conduction band (high energy peak in Figure 3a). While the tunability of the luminescence is the most remarkable process that takes place in Zincblende GaAs under strain, Wurtzite GaAs shows a richer physics. We demonstrated for the first time that uniaxial strain can be used to induce a transition on the band structure from a direct bandgap to a pseudodirect bandgap configuration. In the latter, which is characteristic of Wurtzite crystals, the semiconductor shares some of the properties of direct bandgap and some of indi-

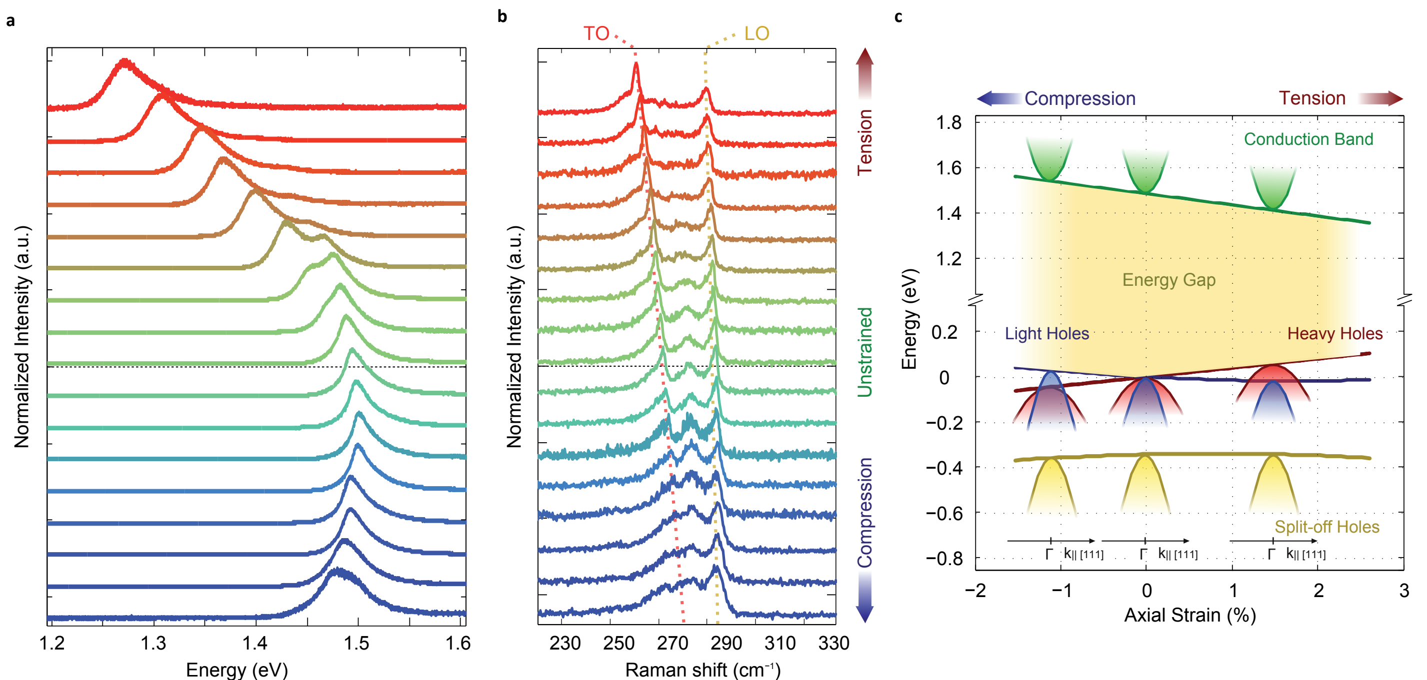

Figure 2. Effect of tensile and compressive stress on the optical properties of the core–shell GaAs–$Al_{0.3}Ga_{0.7}$As–GaAs nanowire. (a) PL spectra measured for different values of applied uniaxial stress. Under compression, the peak shifts weakly and nonlinearly with increasing stress, whereas under tension, a peak splitting is observed together with a strong red shift for the low-energy contribution. (b) Normalized Raman spectra of the GaAs-like phonons (230–330 cm^{-1}) for different values of uniaxial stress. All Raman peaks are observed to shift linearly with stress to higher wavenumbers under compression and to lower wavenumbers under tension. A guide to the eye is included for the peak position of the transversal optical (TO) and longitudinal optical (LO) of the GaAs core. (c) Expected shift of the conduction and valence band edges according to an 8-band k·p model. Heavy-hole band (red) and conduction band (green) edges shift linearly in energy with opposite slope. The light-hole band (blue) energy follows a quadratic dependence on uniaxial stress because of strain mediated spin–orbit interaction with the split-off band (yellow). The small bandgap variation under compression is due to a similar shift of the light-hole band and the conduction band in this stress regime. The substantial red shift observed under tension is related to the change in the symmetry character of the highest energy valence band from light-hole to heavy-hole type.

rect bandgap materials. The relation between energy and wave-vector is indistinguishable from the one of direct bandgap materials: the conduction band minimum and valence band maximum are located at the Γ-point and the respective wavefunctions overlap strongly in the wave-vector space. However, because of symmetry reasons, the optical dipole transitions between these states occur with low probability. The material is therefore a poor light emitter, like indirect bandgap materials. Leveraging on the strain degree of freedom, we have shown that both direct and pseudodirect bandgap configurations can be achieved using a Wurtzite GaAs nanowire (Figure 3c). When tensile stress is applied, the direct configuration can be obtained and the nanowires emit light efficiently; upon compression, the pseudodirect configuration is achieved and light emission can be suppressed by more than three orders of magnitude. The splitting between the dark and bright conduction bands could be tuned continuously over a range of more than 230 meV. Using the Raman scattering spectra as relative strain gauge (Figure 3b) and fitting the optical transition energies to the k·p model, we were able to determine all band structure parameters of the Wurtzite GaAs nanowire in unstrained conditions, i.e., the crystal field (197 meV ± 50 meV) and spin-orbit splitting (293 meV ± 129 meV), the bandgap (1.41 eV ± 8 meV) and, most importantly, the splitting between the bright and the dark conduction bands (33 meV ± 47 meV). Mechanical properties, such as the Poisson ratio along the c-axis (0.17 ± 0.17), and the phonon deformation potentials of the GaAs and AlGaAs optical phonons have also been determined.

These results constitute a solid foundation to the understanding of strain effects on the optical and electronic properties of III-V nanowires. Their implications promise to have high technological relevance, for GaAs and other III-V nanowire electronic and optoelectronic devices.

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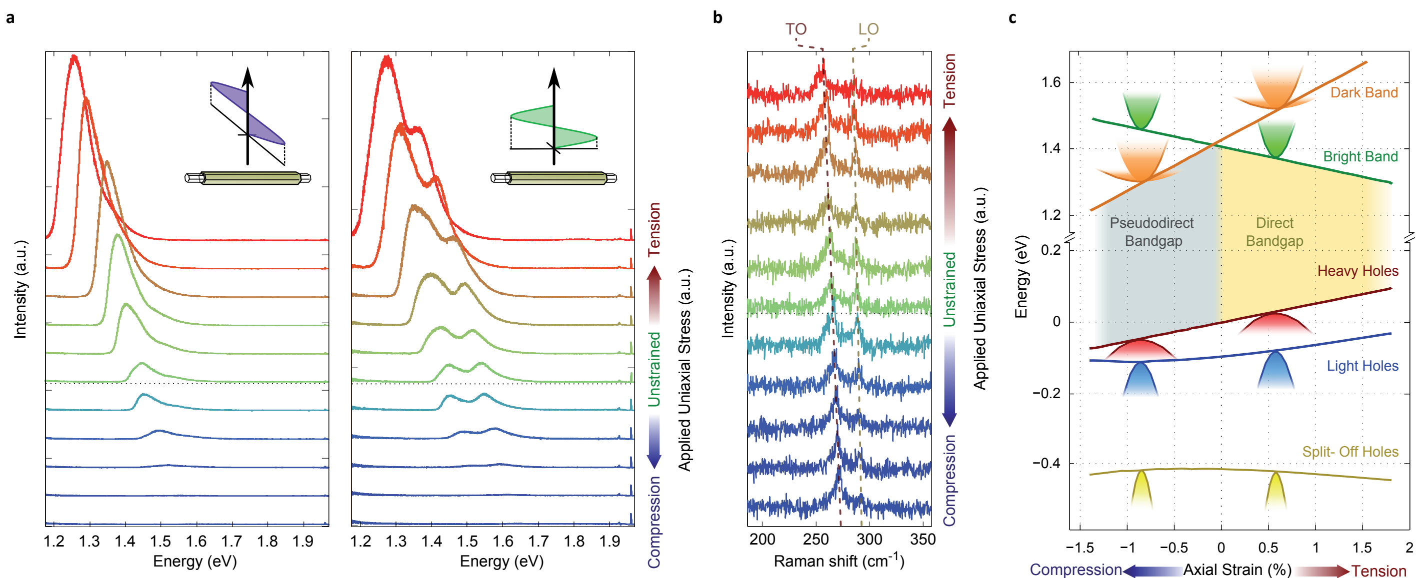

Figure 3. Uniaxial stress effects in Wurtzite GaAs nanowires. Optical spectra collected from a strained Wurtzite GaAs nanowire. The spectra acquired with increasing tensile stress are shown in red, those acquired with increasing compression in blue. The spectra shown in green close to the dashed line are collected without any strain applied. (a) PL spectra acquired with polarization orthogonal and parallel to the nanowire axis are shown in the centre and right panel, respectively. The analyzer configuration is sketched in the inset of each panel. (b) The Raman spectra are shown in the left panel and have been collected with both the laser and the detector polarization aligned with the nanowire axis (scattering configuration not shown). The dotted lines are a guide-to-the-eye to indicate the positions of the phonon peaks attributed to the GaAs transversal optical (TO) phonon with symmetry A1 and the longitudinal optical (LO) phonon with symmetry E1. (c) A 10 band k·p model of the uniaxial stress effects in Wurtzite GaAs. Heavy holes (in red) shift linearly towards higher energies when tensile stress is applied. Light holes (shown in blue) and crystal-field split-off holes (shown in yellow) are coupled by the spin–orbit interaction and undergo nonlinear shifts. In the conduction band, the bright band shifts linearly towards lower energies because of the isotropic component of tensile strain. The dark conduction band shifts towards lower energies under stress, with opposite direction compared to the bright conduction band. The nanowire band structure has a direct bandgap configuration (shaded area in yellow) when the bright conduction band has the lowest energy, and a pseudodirect bandgap configuration (shaded area in grey) when the dark conduction band is lowest. The direct-to-pseudodirect transition occurs when compressive stress is higher than 0.12%.