Effect of Internal Electric Fields on Electronic Transitions in Bent GaAs Nanowires

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Flexoelectricity is an effect that occurs in all dielectric materials under strain gradients, but its influence on the electronic transitions of semiconductors has not been studied experimentally. Here, we exploit the pronounced strain gradient in bent GaAs nanowires (NWs) to investigate this effect by photoluminescence (PL) spectroscopy. In such structures, the combination of strain and strain gradients influences the band gap and induces electric fields originating from both, the piezo- and flexoelectric effect. We analize these contributions in a combined experimental and theoretical study.

We grow self-assembled GaAs NWs which have such a low degree of polytypism that their low-temperature PL spectra exhibit only two transitions characteristic of zincblende GaAs [1]. The remarkable absence of additional low-energy peaks typical for GaAs NWs and related to variations in crystal stacking enables the analysis presented here. Bending results from the deposition of an asymmetric $In_{0.5}Al_{0.5}As$ stressor shell [2]. For a given NW length, the curvature depends on both the NW diameter and the stressor shell thickness, and we adjust both parameters independently.

The PL spectra of single bent NWs show a single peak. The evolution of its position with excitation is compared in Fig. 1 with the position of the free exciton X_{hh} transition in single straight NWs with the same diameter. At the lowest excitation density, there is a strong red shift. The strain gradient across the NWs gives rise to a gradient in band gap via the deformation potential interaction. Thus, charge carriers recombine at the position of highest tensile strain. However, quantitatively the observed red shift cannot be explained by the change of the band gap due to strain alone. This discrepancy and the blue shift of the transition in bent NWs with increasing excitation density indicate the presence of electric fields across the NW that are caused by piezo- and flexoelectricity and spatially separate electrons and holes. With increasing excitation density, these fields are progressively screened by photogenerated carriers.

To analize the different effects in bent NWs, we employ a simple model that computes the energy of the X_{hh} transition on the basis of the change in band gap and the piezo- as well as flexoelectric potential. The band gap gradient follows directly



Fig. 1. Free-exciton X_{hh} peak position of single straight and bent NWs with same diameter. Different symbols correspond to different single NWs. The curvature of all bent NWs is the same. The dashed line presents the X_{hh} position in bulk GaAs and the dotted line the red-shift calculated with our model. The inset shows the scanning electron micrographs of straight and bent GaAs NWs.

from the strain gradient deduced from the observed bending. Furthermore, we extract the magnitude of the piezoelectric contribution from finite element method (FEM) calculations of the maximum piezoelectric field in the bent NWs. To account for the flexoelectric field, we use a simple estimate of the flexoelectric constant, and we compare the overall modelling with the experimental data.

In conclusion, we present a first experimental study taking into account flexoelectricity in GaAs. More generally, the strain gradients in controllably bent NWs can be considered a new level of strain engineering as a means to tailor the electronic properties of semiconductors. References

[1] M. Oliva et al., ACS Appl. Nano Mater. 6, 15278 (2023)

[2] R. Lewis *et al.*, Nano Lett. **18**, 2343 (2018).