Wave-function engineering in $In_{0.53}Ga_{0.47}As/In_xAl_{1-x}As$ core/shell nanowires

Oliver Marquardt
Weierstraß-Institut für Angewandte Analysis und Stochastik, Leibniz-Institut im Forschungsverbund Berlin e.V.,
Mohrenstraße 39, 10117 Berlin, Germany
Email: oliver.marquardt@wias-berlin.de
Lutz Geelhaar and Oliver Brandt
Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V.,
Hausvogteiplatz 5–7, 10117 Berlin, Germany

***Abstract*—We study the electronic properties of $In_{0.53}Ga_{0.47}As/In_xAl_{1-x}As$ core/shell nanowires for light emission in the telecommunication range. In particular, we systematically investigate the influence of the In content x of the $In_xAl_{1-x}As$ shell and the diameter d of the $In_{0.53}Ga_{0.47}As$ core on strain distribution, transition energies, and the character of the hole wave function. We show that the character of the hole state, and thus the polarization of the light emitted by such core/shell nanowires, can be easily tuned via these two experimentally accessible parameters.**

I. Introduction

The materials system (In,Ga)As/(In,Al)As is one of the prime contenders for light emission and absorption in the telecommunication C band at 1.55 μm [1], [2]. Planar (In,Ga)As/(In,Al)As heterostructures may be synthesized perfectly lattice matched to InP substrates, but also with intentionally strained (In,Ga)As layers by detuning their composition. The resulting biaxial strain enables valence-band engineering [3] with beneficial consequences for the characteristics of laser diodes [4]. In this context, core/shell nanowires are of interest since they offer the possibility to incorporate significantly higher levels of strain [5]. In addition, the core diameter can be reduced to values at which strong quantum confinement sets in [6]. Four experimental parameters (core diameter, shell thickness, and the composition of core and shell) are available for controlling the emission wavelength, the strain state of core and shell and thus the ordering of the valence bands, and the degree of quantum confinement. Hence, (In,Ga)As/(In,Al)As core/shell nanowires are highly versatile structures whose properties can be tailored exactly according to the requirements of the specific application. Here, we present a detailed theoretical analysis of the elastic, electronic, and optical properties of $In_{0.53}Ga_{0.47}As/In_xAl_{1-x}As$ core/shell nanowires. We show that both transition energies as well as the character of the hole state can be tuned via the core diameter and the shell In content.

II. Strain distribution and band properties

The elastic properties of the system under consideration, their impact on the electronic properties and finally electron and hole ground state energies and wave functions were computed using the generalized continuum elasticity and multi-band $\mathbf{k}\cdot\mathbf{p}$ modules of the Sphinx physics library [7], [8], [9]. The respective parameters were taken from Ref. [10] and we have employed symmetry-adapted elastic tensor, polarization vector [11], and eight-band $\mathbf{k}\cdot\mathbf{p}$ model [12].

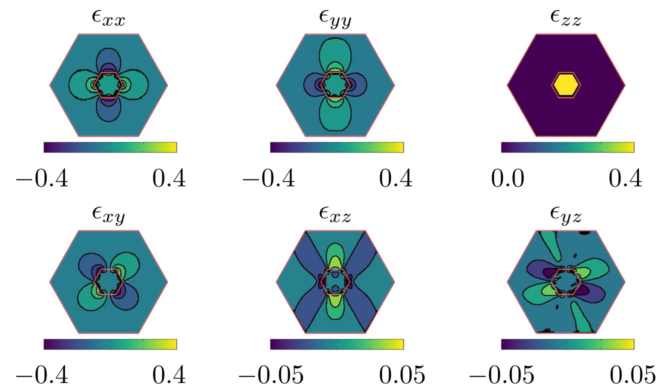

Fig. 1. Strain distribution throughout the nanowire's cross section for a core diameter of 30 nm and a shell In content of $x = 0.6$ in %.

Figure 1 shows the strain distribution throughout the cross-section of an $In_{0.53}Ga_{0.47}As/In_xAl_{1-x}As$ core/shell nanowire with a shell thickness of 50 nm for a shell In content of 0.6 and a core diameter of 30 nm. The magnitudes of the strain are generally in a range that can be elastically relaxed in such systems (in the specific example below 0.4%), but will influence the electronic properties.

In fact, we observe significant alterations of the conduction and valence band edges in the center of the nanowire, as is shown in Fig. 2. While the conduction band decreases by about 300 meV when increasing the In content from 25 to 80%, the valence bands change order at an In content of 53% with the light hole band dominating below and the heavy hole band above this value.

III. Optoelectronic properties

Figure 3 (top) shows the energy difference between electron and hole ground state as a function of the In content x of the $In_xAl_{1-x}As$ shell for core diameters of 10, 20, and 30 nm.

978-1-6654-1276-6/21/$31.00 ©2021 IEEE

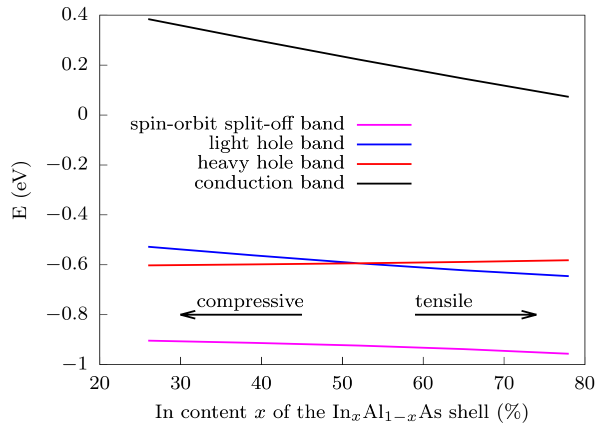

Fig. 2. Band edges in the center of the nanowire's core as a function of the In content x of the shell for a core diameter of d =10 nm.

The thickness of the $In_xAl_{1-x}As$ shell is 50 nm and the core material is $In_{0.53}Ga_{0.47}As$ in all cases. The energies decrease almost linearly below In contents of 50–75%, where a kink towards a stronger decrease of the energies is observed. For the selected core composition, the transition energies cover the entire long-wavelength telecommunication range between the O and the L band.

Figure 3 (bottom) shows the geometrical electron-hole ground state overlap

$$\mathcal{O} = \sum_{r_1}\sum_{r_2}\sum_{r_3} \varrho_{\mathrm{e}}(r_1, r_2, r_3)\varrho_{\mathrm{h}}(r_1, r_2, r_3) \qquad (1)$$

with $\varrho_{\mathrm{e}}(r_1, r_2, r_3)$ and $\varrho_{\mathrm{h}}(r_1, r_2, r_3)$ being the electron and hole ground state charge densities and r_1, r_2, r_3 denoting the spatial discretization of the super cell. The curves exhibit a nontrivial behavior, resulting from the nodal character of the hole wave function (insets in Fig. 3 show the hole charge density). $\mathcal{O}$ increases first, with the hole being of predominantly heavy-hole character, and decreases above a shell In content of $\approx$ 50% for d = 20 and 30 nm, where the hole state is affected by strong band mixing. Above In contents of 60 (at d = 30 nm) or 65% (d = 20 nm) the overlap increases again with the hole being mainly of light-hole character. Finally, $\mathcal{O}$ sharply drops to much lower values due to the hole state being pulled out of the core region by the strong polarization potentials. We note that the intermediate state in which the hole is subject to band mixing is not observed for a core diameter of 10 nm.

IV. Summary

We have investigated the influence of core diameter and shell In content on the optoelectronic properties of $In_{0.53}Ga_{0.47}As/In_xAl_{1-x}As$ core/shell nanowires. These two parameters were found to largely control both the transition energy and the valence band ordering, i. e., the predominant character of the hole state. Tuning them allows us to adjust the transition energy to the desired telecommunication wavelength, and to control the polarization state of the emitted light.

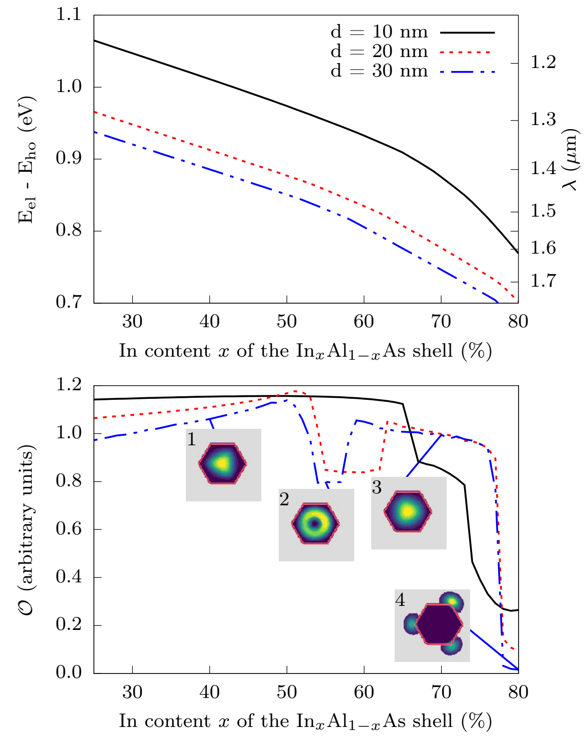

Fig. 3. Top: Electron-hole ground state recombination energy as a function of x for different core diameters d. Bottom: Electron-hole ground state geometrical overlap $\mathcal{O}$ for different core diameters as a function of the shell In content x. A cross-section view of the hole ground state is provided as insets for the characteristic cases.

V. Funding

O.M. is funded by the Deutsche Forschungsgemeinschaft under Germany's Excellence Strategy EXC2046: MATH+ Berlin Mathematics Research Center (Project AA2-15).

References

[1] H. Temkin, K. Alavi, W. R. Wagner, T. P. Pearsall, and A. Y. Cho, Appl. Phys. Lett. **42**, 845 (1983).
[2] S. A. Nazib, T. Hutchins-Delgado, D. M. Contreras, H. Lee, E. J. Charles, N. J. Withers, S. J. Addamane, E. J. Renteria, J. Nogan, G. Balakrishnan, and M. Osiński, Proc. SPIE 10912, Physics and Simulation of Optoelectronic Devices XXVII, 109120X (2019).
[3] E. P. O'Reilly, Semicond. Sci. Technol. **4**, 121 (1989).
[4] E. S. Kolodeznyi, I. I. Novikov, A. V. Babichev, A. S. Kurochkin, A. G. Gladyshev, L. Ya. Karachinsky, I. M. Gadzhiev, M. S. Buyalo, A. A. Usikova, and N. D. Ilynskaya, J. Phys.: Conf. Ser. **917**, 052021 (2017).
[5] L. Balaghi, G. Bussone, R. Grifone, R. Hübner, J. Grenzer, M. Ghorbani-Asl, A. V. Krasheninnikov, H. Schneider, M. Helm, and E. Dimakis, Nature Comm. **10**, 2793 (2019).
[6] B. Loitsch, D. Rudolph, S. Morkötter, M. Döblinger, G. Grimaldi, L. Hanschke, S. Matich, E. Parzinger, U. Wurstbauer, G. Abstreiter, and G. Koblmüller, Adv. Mater. **27**, 2195 (2015).
[7] *sxrepo.mpie.de*
[8] S. Boeck, C. Freysoldt, A. Dick, L. Ismer, and J. Neugebauer, Comp. Phys. Commun. **182**, 543 (2011).
[9] O. Marquardt, S. Boeck, C. Freysoldt, T. Hickel, S. Schulz, J. Neugebauer, and E. P. O'Reilly, Comp. Mat. Sci. **95**, 280 (2014).
[10] I. Vurgaftman, J. R. Meyer, and L. R. Ram-Mohan, J. Appl. Phys. **89**, 5815 (2001).
[11] S. Schulz, M. A. Caro, E. P. O'Reilly, and O. Marquardt, Phys. Rev. B **84**, 125312 (2011).
[12] O. Marquardt, E. P. O'Reilly, and S. Schulz, J. Phys.: Condens. Matter **26**, 035303 (2014).