Electronic properties of polar and semi-polar dot-in-a-well heterostructures

Stefan Schulz
Tyndall National Institute
Lee Maltings, Cork, Ireland
Email: stefan.schulz@tyndall.ie
Oliver Marquardt
Paul-Drude-Institut für Festkörperelektronik
Hausvogteiplatz 5–7, 10117 Berlin, Germany
Email: marquardt@pdi-berlin.de

***Abstract*—We use a symmetry-adapted formalism to compute the elastic, piezoelectric, and electronic properties of polar and semi-polar dot-in-a-well (DWELL) systems. Our simulations reveal a reduced spatial separation of electron and hole ground state wave functions in semi-polar DWELL systems compared to their polar counterparts. This originates in part from the strongly reduced built-in potentials and in part from changes in the built-in potential profile. Our findings thus indicate superior recombination rates of semi-polar DWELLs, making these systems highly promising for future optoelectronic devices.**

I. Introduction

The optical properties of III-nitride semiconductor heterostructures grown on polar substrates suffer significantly from strong built-in fields, leading to a large spatial separation of electron and hole wave functions and thus to strongly reduced recombination rates [1]. The growth of heterostructures on semi- or nonpolar substrates represents an attractive alternative and much research effort has been dedicated towards semi- and nonpolar quantum well (QW) heterostructures, recently [2], [3], [4], [5]. However, these systems exhibit a high density of extended defects, giving rise to unwanted nonradiative recombination [6]. This problem can be potentially solved by embedding quantum dots (QDs) in semi- and nonpolar QWs, thus forming dot-in-a-well (DWELL) heterostructures. In fact, this concept has been successfully applied in $In_xGa_{1-x}As$-based devices in the past, yielding improved device performance in the spectral range of 1200 – 1400 nm [7], [8].

In the present work, we transfer this DWELL concept to $In_xGa_{1-x}N/GaN$ heterostructures grown on polar and semi-polar substrates and compare these systems. For this purpose, we have employed symmetry-adapted formalisms to compute elastic, piezoelectric, and electronic properties. We show that, when varying the In content in the QD (c_d) and in the QW (c_w), $In_{c_d}Ga_{1-c_d}N/In_{c_w}Ga_{1-c_w}N$ DWELL heterostructures grown on $(11\bar{2}2)$-oriented semi-polar substrates exhibit in comparison with their polar counterparts superior ground state wave function overlaps. This indicates that semi-polar DWELLs can be considered as promising candidates for future optoelectronic devices.

II. Impact of QD and QW In content

We study a lens-shaped $In_{c_d}Ga_{1-c_d}N$ QD of a diameter of 10 nm and a height of 2.5 nm, embedded in an $In_{c_w}Ga_{1-c_w}N$ QW of a thickness of 4.5 nm. For the sake of comparability, we assume identical shapes and dimensions for both polar and semi-polar systems. To compute elastic, piezoelectric, and electronic properties of these DWELLs, we have employed a symmetry-adapted $\mathbf{k}\cdot\mathbf{p}$ model [9]. All required ingredients, such as stiffness tensor, piezoelectric polarization vector field and (strain-dependent) Hamiltonian, were derived analytically as a function of the inclination angle θ to the [0001]-direction. The formalism was implemented within the S/Phi/nX software library [10], [11].

We have computed strain distribution, built-in electric field, electron and hole ground state energies and wave functions. Based on the single-particle properties, the oscillator strength f^λ can be determined as:

$$f^\lambda = \frac{2}{m_0\hbar\omega}\left|\langle\Psi_{\mathrm{el},\lambda}|\mathbf{e}\cdot\mathbf{p}|\Psi_{\mathrm{ho},\lambda}\rangle\right|^2 \quad (1)$$

where λ=(p) or (sp) denotes polar or semi-polar structures, $\mathbf{p}$ is the momentum operator, and $\mathbf{e}$ denotes the light polarization vector. Here we use $\mathbf{e}=1/\sqrt{2}(1,1,0)^T$. We then determine $\tilde{f}^\lambda$ as a normalized oscillator strength where the reference is the oscillator strength of an isolated polar $In_{0.25}Ga_{0.75}N/GaN$ QD. In the following, we focus on an $In_{0.25}Ga_{0.75}N$-QD embedded in an $In_{c_w}Ga_{1-c_w}N$-QW within a GaN host matrix. We discuss the localization of electron and hole ground state wave function and (normalized) oscillator strengths as a function of the QW In content, c_w.

Figure 1 shows the electron and hole ground state charge density for the polar (top) and the semi-polar (bottom) DWELLs for QW In contents of c_w=0, 0.05, and 0.10. The In content in the dot is again fixed at c_d=0.25. For the polar DWELL, the well-known strong spatial separation of electron and hole wave function along the growth direction, resulting from the large built-in potential [12], is seen for all QW In contents c_w. This separation increases even further when increasing c_w, as the higher QW In content leads to larger built-in potentials. For $c_w=0.1$, both electron and hole are

978-1-4799-8379-7/151$31.00 ©2015 IEEE

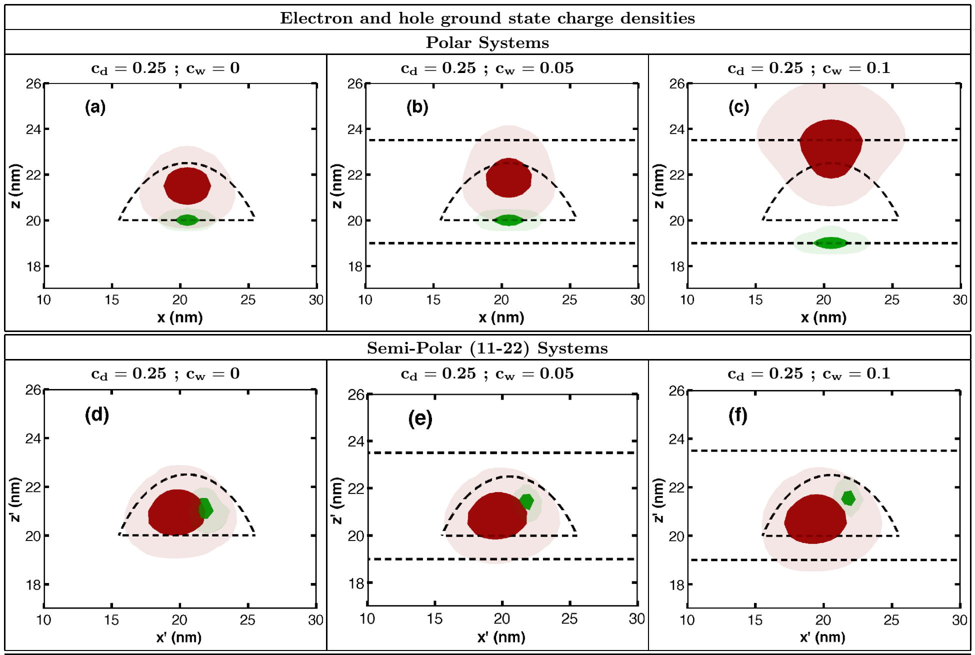

Fig. 1. Electron (red) and hole (green) ground state charge densities in polar (top) and semi-polar (bottom) DWELLs for different In contents of the well surrounding an $In_{0.25}Ga_{0.75}N$/GaN QD. Dashed lines indicate QD and well interfaces.

localized outside the QD already. In the semi-polar DWELL, a smaller spatial separation is observed. Note, this separation is not aligned with the $[11\bar{2}2]$ growth direction, but rather within the [0001]-direction. With increasing In content of the QW, the spatial separation of electron and hole is increased, but still much smaller than in the respective polar system. The corresponding normalized oscillator strength $\tilde{f}^{\lambda}$ is shown in Fig. 2 for the polar (black solid) and the semi-polar (dashed red) DWELL. As discussed above, the normalization is done here with respect to an isolated polar $In_{0.25}Ga_{0.75}N$-QD. When comparing isolated QDs on polar and semi-polar substrates, we find the oscillator strength of the semi-polar system to be four times larger than the one of the polar QD. For both polar and semi-polar DWELLs, the oscillator strength is reduced with larger QW In content c_w, as the spatial separation of electron and hole wave function is increased in both systems. Nevertheless, the oscillator strength of the semi-polar DWELL is always much larger than the one of the polar DWELL, and for a QW In content of 10%, $\tilde{f}^{sp}$ is almost as large as the oscillator strength of an isolated polar QD (cf. Fig. 2).

In summary, we find that semi-polar DWELLs exhibit much larger spatial electron and hole ground state wave function overlaps than equivalent polar DWELLs. This makes semi-polar DWELL systems highly attractive for novel III-nitride based light emitters.

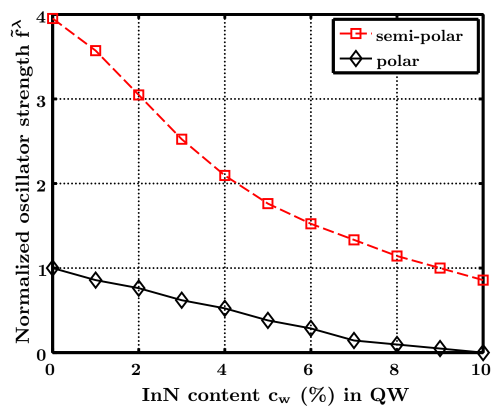

Fig. 2. Normalized oscillator strength in polar (black solid) and semi-polar (red dashed) $In_{0.25}Ga_{0.75}N$ QDs embedded in QW as a function of the In content of the QW, c_w.

REFERENCES

[1] F, Widmann, J. Simon, B. Daudin, G. Feuillet, J. L. Rouvière , N. T Pelekanos, and G. Fishman, Phys. Rev. B **58**, R15989 (1998).
[2] P. Waltereit, O. Brandt, A. Trampert, H. T. Grahn, J. Menninger, M. Ramsteiner, and K. H. Ploog, Nature **406**, 865 (2000).
[3] U. T. Schwarz and M. Kneissl, Phys. Stat. Sol. (RRL) **1**, A44 (2007).
[4] Y. Zhao, S. Tanaka, C. C. Pan, K. Fujito, D. Feezell, J. S. Speck, S. P. DenBaars, and S. Nakamura, Appl. Phys. Express **4**, 082104 (2011).
[5] O. Marquardt, T. Hickel, J. Neugebauer, and C. G. Van de Walle, Appl. Phys. Lett. **103**, 073115 (2013).
[6] J. Abell and T. D. Moustakas, Appl. Phys. Lett. **92**, 091901 (2008).
[7] K. B. Hong and M. K. Kuo, Semicond. Sci. Technol. **28**, 105006 (2013).
[8] M. T. Crowley, S. C. Heck, S. B. Healy, S. Osborne, D. P. Williams, S. Schulz, and E. P. O'Reilly, Semicond. Sci. Technol. **28**, 015012 (2013).
[9] S. Schulz and O. Marquardt (submitted).
[10] S. Boeck, C. Freysoldt, A. Dick, L. Ismer, and J. Neugebauer, Comp. Phys. Commun. **182**, 543 (2011).
[11] O. Marquardt, S. Boeck, C. Freysoldt, T. Hickel, S. Schulz, J. Neugebauer, and E. P. O'Reilly, Comp. Mat. Sci. **95**, 280 (2014).
[12] J. Simon, N. T. Pelekanos, C. Adelmann, E. Martinez-Guerrero, R. Andre, B. Daudin, L. S. Dang, and H. Mariette, Phys. Rev. B **68**, 035312 (2003).