Theoretical correlation between quantum dot composition and polarization properties

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Quantum dot nanostructures have been extensively studied for several applications involving design of optoelectronic devices, single photon sources, entangled photon emissions etc. In most of these applications, one crucial parameter is the polarization response that is typically measured in terms of degree of polarization. Understanding how this parameter is related to quantum dot (QD) structural symmetry and composition profile is critical for its tuning. The InAs QDs obtained by the self-ordering Stranski-Krastanov process have been found to be significantly influenced by In-Ga intermixing and In-segregation effects during the capping and post-growth annealing processes. This results in a complex QD composition profile, which is strongly related to the growth conditions. Recent review by Biasiol and Heun (Physics Reports 500, 117-173, 2011) reports a common tendency that the QDs have In rich core at the center with In composition decreasing from center towards edges in the lateral directions. Such a complex composition profile has not been considered so far in theoretical studies of the polarization properties.

Previous theoretical studies are based on a pure InAs type QD composition profile, thus significantly limiting their accuracy and leading to discrepancy between theory and experiment. In this work, we propose a two composition model (figure b) to mimic In-Ga intermixing and In-segregation affects. Based on multi-million atom simulations, we perform a systematic analysis of the dependence of the QD polarization properties on various QD morphology parameters. Our theoretical results accurately reproduce the experimental polarization response and highlight the strong anisotropy of atomic scale phenomena like intermixing and segregation affecting the polarization behavior of these nanostructures. These results could represent a tool for using growth dynamics to engineer the strain field inside and around the QD structures, allowing tuning of the polarization properties, a critical parameter for several challenging applications.