Electronic structure of InN-based nanowires using multiband $\mathbf{k} \cdot \mathbf{p}$ envelope function method

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Group III nitride materials are well known for their excellent optical and electronic properties. Among these compounds, InN possesses the narrowest bandgap, the smallest effective electron mass, and the highest electron mobility. Moreover, the recent advances in the fabrication methods allow the growth of InN, ternary $In_xGa_{1-x}N$, and InGaN/GaN heterostructure in nanowire-like geometry. Due to these unique properties, the wurtzite InN-related nanowires are promising systems for applications in energy harvesting [1] and optoelectronic nanodevices [2].

In general, wurtzite semiconductors have a complicated valence band structure, and in the special case of InN, several studies have reported also a strong non-parabolicity of the conduction band [3]. In the case of InN-based core-shell nanowires, the strain also alters the band structure. All these factors make difficult the analysis of experimental results, and theoretical models are demanded to understand the trends in the electronic and optical properties of nanowires. In this work we propose a multiband $\mathbf{k} \cdot \mathbf{p}$ envelope function method to study the electronic structure of InN-based nanowires. We report on the electronic states, optical matrix elements and optical absorption of infinitely long cylindrical free standing InN nanowires and InN-based core-shell nanowires (see figure below). We present an analysis of the symmetry of the valence and conduction states, as well as the effect of size and strain on the nanowire band gaps.

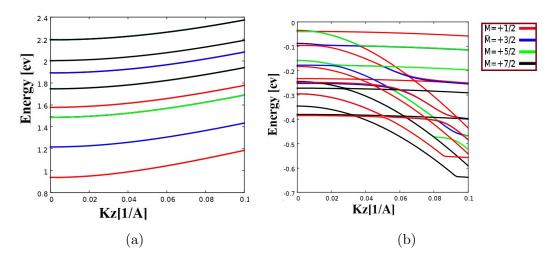


Figure 1: (a) and (b) show conduction and valence bands of cylindrical InN nanowire, R=20 nm

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References

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