Microscopic models of polarization, polarization charges and dipole layers - application to nitride multiquantum wells (MQWs)

Stanislaw Krukowski[1,2], Pawel Strak[1], Pawel Kempisty[1] and Konrad Sakowski[1]

[1] *Institute of High Pressure Physics, Polish Academy of Sciences, Sokołowska 29/37, 01-142 Warsaw, Poland*

[2] *Interdisciplinary Centre for Materials Modeling, University of Warsaw, Pawińskiego 5a, 02-106 Warsaw, Poland*

Microscopic model of polarization in solid is proposed, with special application to wurtzite semiconductors, such as AlN, GaN and InN. It is shown that multiple polarization values are obtained by both approaches: standard based on dipole density and modern based on Berry phase approach. The selection of the proper polarization is dependent on the boundary conditions at polar surfaces. The role of surface charge, i.e. located on surface states and screening, is elucidated with respect to influence on the selection of polarization and the polarization induced electric field. It is shown that the selection of the polarization and the electric field is independent of the size of the polar specimens. The proper application of the boundary conditions leads to selection of single polarization value id dipole formulation. The obtained dipole result will be compared to Berry phase result. The existence of dipole layers is discussed and the conditions of its existence are shown based on microscopic models. The related properties such as potential jumps at heterointerfaces and the band offsets are discussed using DFT simulations of AlN/GaN and GaN/InN multiple quantum wells (MQWs).