On the Applicability of the Theory of Elasticity to Very Thin Layers

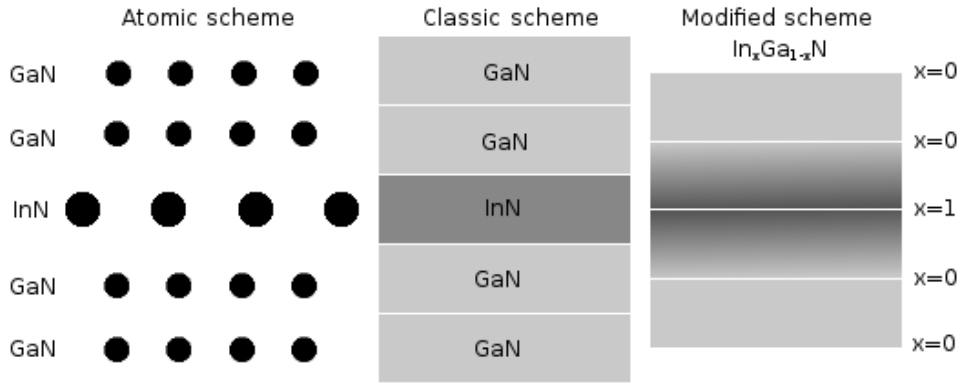
G. Jurczak[1,*], M. Maździarz[1], P. Dłużewski[1],
G. Dimitrakopulos[2], Ph. Komninou[2], and T. Karakostas[2]

[1]Institute of Fundamental Technological Research of the Polish Academy of Sciences, ul. Pawińskiego 5b, 01-494 Warsaw, Poland
[2]Department of Physics, Aristotle University of Thessaloniki, GR 54124 Thessaloniki, Greece

corresponding author: gjurcz@ippt.pan.pl

Theory of elasticity, a continuum model of a macroscopic material is commonly used to model a relaxation of a crystalline heterostructures. There are many reports on the successful application of theory of elasticity to nanometer crystalline heterostructures, even if the continuum condition for these structures is hardly fulfilled. On the other hand progress in epitaxial growth techniques allows to prepare the stable ultra thin layers with the thickness about a single monolayer. For such extremely thin layers the theory of elasticity seems to fail in describing the relaxation process. The results provided by theory of elasticity and experimental measurements or molecular statics/dynamics become diverging. The key problem in that case seems to be located at the interface between layers and related to composition change, which is problematic in classic, elastic approach. By applying a “substitutive” composition of the interface layers which is just an interpolation, it is possible to obtain a good agreement with molecular statics, even for 1 monolayer heterostructure.

Instead of classic approach to the composition within the theory of elasticity, we propose another approach which takes into account the composition as an extra degree of freedom along with classical displacement [1]. Such approach creates a chemo-elastic coupling with composition interpolated by use of the Vegard’s law. This allows to take into account a composition changes at the interface and avoid mesh refining necessary at the classic approach.



[1] P. Dłużewski, G. Maciejewski, G. Jurczak, S. Kret, and J.-Y. Laval, Comput. Mater. Sci. 29, (2004) 379–395.