DFT-based modeling of the point defects migration in the bulk GaN, InN, and AlN crystals

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Group-III nitride semiconductors GaN, InN and AlN are very attractive for a wide application in optoelectronics. Modern light emitting devices utilize these nitrides as the multi-quantum well structures. Efficiency of a light emitting device is still affected by the presence and diffusion of point defects in the nitride heterostructures. In order to explain the decomposition of e.g. InGaN/GaN multi-quantum well structure during its growth and post processing caused by defects, it is necessary firstly to model a diffusion of point defects in bulk nitrides.

Herein, we present theoretical *ab initio* DFT-based calculations of formation energy and heights of energy barriers encountered at the migration of neutral and charged point defects in GaN, InN, and AlN bulk crystals. In particular, we study single vacancies V_N, V_{Ga}, V_{In}, V_{Al}, double vacancies $2V_N$, $2V_{Ga}$, $2V_{In}$, $2V_{Al}$, as well as complex of a substitution atom and metal vacancy $In_{Ga}+V_{Ga}$, $Al_{Ga}+V_{Ga}$, $Ga_{In}+V_{In}$, $Al_{In}+V_{In}$, $Ga_{Al}+V_{Al}$, $In_{Al}+V_{Al}$ in the mentioned above bulk nitrides. Additionally, we investigate various charge state of these defects, which play a roll of potential donors, or acceptors.

By means of the Nudged Elastic Band (NEB) method we estimate heights of diffusion energy barriers that lie in the range of 1.10 – 6.80 eV. We show that (i) migration of a charge defect proceeds with smaller energy barrier than the neutral ones, (ii) energy barrier encountered at the migration of point defect in the lateral directions is smaller than that one in the *c* direction, (iii) energy barriers of 'defect complexes' i.e., substitution atom in the presence of additional metal vacancy, are the smallest in all studied materials.

Acknowledgements: The authors thank the TEAM/2016-3/26 project that is carried out within the TEAM programme of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund.