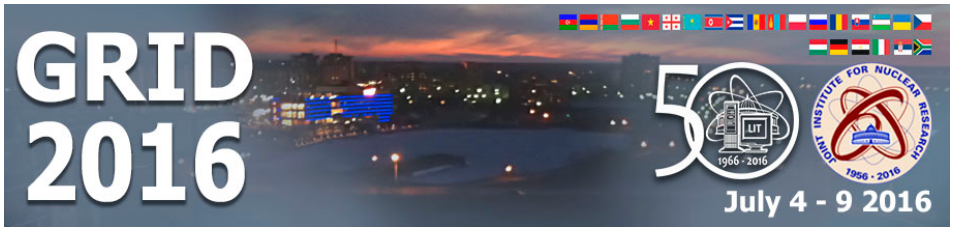

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Parallel algorithms for calculation of binding energies and adatom diffusion on GaN (0001) surface

Tuesday, 5 July 2016 16:00 (15 minutes)

Empirical many-body potentials were used to calculate the binding energies and diffusion barriers for various adatoms on the GaN (0001) surface. Potential energy surfaces were calculated for adatoms by letting them relax in c-direction on Ga terminated (0001) surface of GaN. The minimum energy positions for Ga and N adatoms on the Ga-terminated GaN (0001) surface were identified. This allowed determination of the diffusion pathways and the diffusion barriers for adatoms. Parallel GPGPU computing was performed for the acceleration of empirical potentials and the algorithms of energy minimization. OpenCL technology was used to support both CPU and GPU computing. The basic results were compared with DFT calculations for the same structures. It was shown that Tersoff and Stillinger-Weber empirical potentials do not reproduce correctly the minimum energy positions of adatoms on GaN (0001) surface. Additional potential fitting is required to reproduce binding energies and diffusion barriers. Interatomic potential fitting and potential energy surface calculation are the problems to be done in parallel by high performance hardware or GRID infrastructure.

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