Copyright © 2008 ICCES Proceedings of ICCES'08, pp.873-873

Pseudoperiodic Simulation of Nanostructures

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Summary

We have devised a pseudoperiodic model for the simulation of nanostructures. In this model, a finite periodic nanocrystal is mapped onto the nanostructure geometry, greatly reducing the degrees of freedom required for energy optimizations. The current implementation neglects geometric surface relaxation and employs an atomistic pair potential energy model. As a first application of the model, we have simulated nanobelts and nanorings of AlN, both in the wurtzite-like B4 phase and in the rocksalt-like B1 phase. The latter are assumed to present [100] facets in the nanostructure, while the former are simulated with the experimentally found morphology. The focus has been in the size evolution of the properties, and hence nanostructures from 8 to 80000 atoms have been computed. We have explored the infinite-size limits and their thickness evolution as a test of the validity of the model. Our results compare the relative stability of the different phases on the two nanostructure classes, together with the nanobelt-nanoring interconversion equilibrium.

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