 Proceedings of ICCES'08, pp.871-871

Simulation of thermodynamic properties in AlN nanocrystals

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Summary

We present the periodic cluster model, a theoretical scheme recently developed in our laboratory, and use it to simulate thermodynamic properties of AlN nanocrystals within an atomistic pair potential energy model. The main advantages of this approach are a greatly reduced dimensionality and the ability to incorporate external pressure effects, at the cost of neglecting geometric surface relaxation.

The results suggest that small-size nanocrystals display graphitic-like layers, non-buckled, as opposed to the buckled bulk wurtzite structure; buckling will dominate after a given, quite large, threshold. The surface tension, c/a ratio, and equation of state are examined both with respect to variations on pressure and nanocrystal size. It is found that, although the bulk modulus of the wurtzite-like phase is smaller (although decreasing with size) in nanocrystals than in the bulk, the non-buckled phase displays a quite larger bulk modulus, in agreement with the experiments. The transition pressure into the rocksalt-like phase increases with system size, the dependence being linear against $1/N^{1/3}$. This is rationalized through a qualitative small-systems thermodynamical model.

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