On structural and electronic properties of small silicon nanoclusters

V. S. Baturin[1], S. V. Lepeshkin[1], N. L. Matsko[1], Yu. A. Uspenskii[1]

[1]*P.N. Lebedev Physical Institute, Russian Academy of Sciences, 119991 Moscow, Russia*

The small nanoclusters are very promising objects for the development of opto- and nanoelectronics, mostly because of their compatibility with currently dominating silicon-based technology of microelectronics. In this regard, the problem of production clusters with predetermined features is crucial. Since physical properties are determined by structure, a lot of effort had been put to develop methods of finding low-energy structures of atomic systems.

For large clusters (with sizes >5nm) it is well known experimentally, that their core has the structure of bulk sample, but for small ones the arrangement of atoms strongly depends on number of atoms.

In present work we will focus on the global optimization method based on combining evolutionary algorithms with sequential refinement of atomic interaction models. We use the USPEX code as the implementation of evolutionary algorithm for it has proved to be successful in solving many solid-state problems. [1] This code implies the creation of 'generation' of structures with subsequent local optimization. For this optimization we used the empirical potentials on the first steps of our calculation, and the ab-initio relaxation on the final steps. It allowed to save the CPU time without significant loss of accuracy.

As a result we calculated the stable structures of Si_n with n = 4...13 and of passivated clusters $Si_{10}H_{2m}$ (m=6,8,11). These structures showed excellent agreement with available experimental data [2] and earlier calculations performed by different optimization methods [3]. Further possibilities to accelerate cluster structure prediction are discussed. Authors are grateful to Ministry of Education and Science of Russia, Russian Academy of Sciences, and Russian Foundation for Basic Research for partial support of this research.

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