Quantum Computer Modeling of Realistic Many Body Interatomic Potentials in Nanostructures by Quantum Topological Method of Density Functional Theory

Abstract

We discuss some realistic many body interatomic potentials in nanostructures of atoms localized inside strong correlated quantum wells as a result of the kinematic electron-density waves swarming. A confinement-induced enhancement of the electron-electron interaction may be responsible for the change of interactions between atoms inside nanosystem. Using computer modeling interatomic potentials were obtained for 3D nanosystems of Al and Si.

Keywords: Nanostructure, Quantum Confinement; Density Functional; Computer Simulation

1. Introduction

One of the most fundamental idea is a quantum swarming of atoms within low dimensional superfine channels in nanostructured materials [1,2]. It is a very peculiar quantum effect, in which the quantum electrodynamics is dependent on strong effects of correlation in the electronic medium. Previously, we discussed a model of approximation of 3-dimensional atomic swarm arranged inside nanosystem of interfaces and channels. Now we take under consideration many body interatomic potentials acting between metal atoms (Al) and nonmetal atoms (Si) within homogeneous swarmed quantum mechanical block and some comparison with those in bulk crystals.

*Corresponding author: tel: +7 3852 268744; e-mail: beznosyuk@chemwood.dcn-asu.ru

Differences between two above-mentioned models are exactly defined in the frame of the quantum field chemistry (QFC) approach to problems of quantum electrodynamics in nanostructured materials [1,2]. According to QFC-theory a quantum mechanical simple block does not include any quantum mechanical subblocks and it has got compact domain without mosaic compactly connected set of subdomains. For example, it is a single quantum mechanical particle such as a single crystal. Besides it there are some quantum mechanical mosaic blocks in nanostructured matter. Each of them includes a swarm of quantum mechanical subblocks. In a physical space the mosaic block has got compact topology domain with mosaic compactly connected set of subdomains.

The compact embedded subsystem of nuclei and electrons within each subblock has a subset of local kinematic electron-density waves by itself, which is defined on the compact support of the subdomain. Swarming means that joint mosaic block has entire kinematic electron-density waves also. This part of the collective variables describes compact collective movement of subblocks inside swarm. There is a hierarchy of subdomain and entire domain kinematic electron-density wave subsets. Thus the swarm inside mosaic block domain bears a resemblance to the well-known topology of “Russian doll”.

In fact the above-mentioned models of simple and mosaic blocks represent special extreme solutions of basic QFC- dynamic equation [1]. Preferred solution is determinated with variational minimum of the ground state energy. Special types of electron density functional (DF) constitutes energy of such states. In the swarm block model it is the aproximating quasiparticle density functional (AQDF) for inhomogeneous electron swarm [1,2].

The present paper is organized as follows. In Sec. 2 some new quantum approach to atomic topology of nanosystems are formulated. In Sec. 3 we shortly discuss of computer simulation of a strong correlated potential wells of Al and Si atoms inside nanosystem.

2. Quantum Field Chemistry and Swarm Topology of Nanostructured Materials

One of the most fundamental concepts giving good grounds for theoretical investigation of various nanosystems seems to be the quantum topology [1]. In which using topological property of electron density it was shown that quantum mechanical subsystem of matter could be described as a collection of atoms $\{v_j\}$. Each atom is a basin of density gradient paths attracted to cusp point of density at nuclei. The electron density $n(x)$ distributed in the atomic basin v satisfies two boundary constraints, as follows, the singular cusp-condition by Kato at nuclei and zero-flux gradient density topological condition by Bader on the atomic boundary surface.
It should be noted that a mesa volume W of the condensed state may be represented as topological conjunction of atoms and the environment V[3]:

$$W = V \cup \left(\bigcup_j v_j \right). \qquad (1)$$

In accordance with the quantum field chemistry approach one can define the quantum mechanical N electron compacton as observable in 3D physical space electron domain Ω_m in which electron density distribution $n(x)$ must be described by the condition of the N representability [1]:

$$n(x)\,|_{\Omega_m} \equiv N_m \left| \varphi^1_{0m}(x) \right|^2 . \qquad (2)$$

and depends on set of topological boundary constraints, as follows [1,3]:

$$\vec{\nabla} n(x)\,|_{S_m} = 0; \quad n(x)\,|_{S_m} = n_c. \qquad (3)$$

Every domain is represented by set of some atomic basins closed with a specific subspace of environment $V_m \subset V$, as follows:

$$\Omega_m = V_m \cup \left(\bigcup_{j \in m} v_j \right) \qquad (4)$$

Every compacton has got a special set of collective variables $\{\varphi^1_{qm\tau}(x)\}$ having form of the kinematic electron-density waves, which generalizes of equidensity orbital basis from Harriman [1]:

$$\varphi^1_{qm\tau}(x) = \varphi^1_{0m\tau}(x) \exp\left(i\vec{q}\vec{\Theta}(x; [\varphi^1_{0m\tau}(x)]) \right). \qquad (5)$$

It is a conventional function basis, which is determined on the point lattice of integer numbers in 3D-momentum subspace: $\vec{q} = \sum_{i=1,3} \vec{i} q_i, q_i = 0,\pm1,\pm2,...$.

The quantum mechanical electronic Hilbert space for the mosaic M-block is the linear capsule of antisymmetric products of N-particle kinematic electron-density wave sampling, which is taken from joint set of kinematic electron-density waves, as follows: Thus the swarm has got a quantum mechanical state in a form of linear combination of N-electron configurations. At the same time every N-electron configuration is some Slater's determinant including N ($N = N_M + N_1 + N_2 + \ldots + N_B$) kinematic electron-density waves. The compacton is created within some domain only as a result of total minimization of ground state energy. Each of the order parameters $\{\varphi^1_{0m\tau}(x)\}$of electron τ-phase transitions inside compacton domain can be obtained with the self-consistent variational procedure for the ground state energy, which is an functional of $\varphi^1_{0m\tau}(x)$ [1]:

3. Many Body Interatomic Potentials in Swarming Nanosystems of Al and Si.

There are some atoms of greatest importance to nanomechanical design: carbone, silicon and their neighbors in Periodic table of the atoms: B, N, and Al, P.Computer modeling of interatomic potentials for nonmetal, metal and adhesive bonded atoms in nanosystem reveals very peculiar properties overwhelmingly important for design features. Previously obtained formulas (see [1,2]) have been applied by us to computer simulation of confined many body interatomic potentials in the nanoswarm state of the atomic movements. For example, some selected values of calculated equilibrium parameters of Al and Si domains in nanosystem are given in Tabl. 1. There are some experimantal values of equilibrium parameters for single-crystals. One can see that equilibrium parameters of Al and Si swarming block domains in nanosystem are slightly differ from those which are observed in single crystals.

Table 1
Computing equilibrium parameters of Al and Si atoms and domains in nanosystem

Atom	Ionizing Energy (theory), eV	Ionizing Energy (exp.), eV	Equilibrium bond length (nm)		Equilibrium bond energy (eV/at)	
			Nano-domain (theory)	Crystal (exp.)	Nano-domain (theory)	Crystal (exp.)
Al	6.14	5.99	0.307	0.287	3.08	3.39
Si	8.62	8.15	0.228	0.235	5.25	4.64

Conclusions

From the above we see that a confinement-induced enhancement of the electron-electron interaction is, in principle, responsible for inducement of some new "metal-metal" and "nonmetal-nonmetal" many body interatomic potentials. Swarming of the single atoms within nanosystems makes some nontrivial changes in the well-known interatomic potentials, which observed, as usually, in the ground state of single crystal.

Acknowledgments

Financial support of this scintific program from the Department of Education of Russian Federation is gratefully acknowlodged.

References

[1] S.A. Beznosjuk, B.F.Minaev, R.D. Dajanov, Z.M. Muldakhmetov, Int. J. Quant. Chem., vol.38, No. 6, 1990, pp. 779-797.
[2] S.A. Beznosjuk, R.D. Dajanov, A. T. Kuldjanov, Int. J. Quant. Chem., vol.38, No. 5, 1990, pp. 691-698.
[3] S.A. Beznosjuk, Russian Physics Journal, vol.39 No. 5, 1996, pp 492-503.