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Theory and Computer Simulation of Quantum NEMS Energy Storage in Materials

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The theory of quantum relaxation of the nanoelectromechanical system (NEMS) energy storage in materials is taken under consideration. By using the method of quantum NEMS kinetics (NK) the relaxation NEMS energy storage in the form of limited planes (100) Fe_{172} cube in fcc iron crystal was studied. For comparison, the calculation a similar structure atomic cluster Fe_{172} was carried out by the molecular dynamics method (MD) for temperature T = 293 K. Analysis of computer-related experiments have shown that the relaxation of the NEMS energy storage Fe_{172} and the MD atomic cluster Fe_{172} from an initial nonequilibrium state has significant differences both in the kinetics, and in a variety of structural transformations. It is shown that the iron MD cluster relaxation is insignificant and its final total binding energy per atom is 2 eV/at lower than the crystal one. The NK-method revealed that after relaxation there is a significant change in the shape and the pair radial distribution function of nuclei the NEMS energy storage. It significantly increases the binding energy up to 3.34 eV/at, which is only about 1 eV/at less than the binding energy of the crystalline iron. It is shown an opportunity to undergo a process of self-organization the NEMS energy storage through several intermediate metastable states. It is manifested that fluctuation rebuild the cube into a cuboid with a strong bending of the cube surfaces occurs at 20 ps of relaxation, and there is the second transformation being with trapezoid change of faces at 40 ps of relaxation process. This effect cardinally differentiates NK relaxation of the NEMS energy storage cube Fe_{172} from MD relaxation of the atomic cluster Fe_{172} in the crystalline iron.

Keywords: Quantum NEMS; energy storage; iron cluster; computer simulation.

1. Introduction

The development of modern high-tech demands of the miniaturization of functional electronic elements to the size of less than ten nanometers, the creation high volume capacity nano-accumulators of active hydrogen, engineering of quantum nanoelectromechanical system (NEMS) robotics, the development of low power pulsed lasers in the hard ultraviolet and soft X-rays. These and many other problems still hampered by lack of precise

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understanding of the mechanisms of superdense energy storage in small quantum-sized nanoparticles of materials. These include, in particular, the mechanisms of accumulation and dissipation in condensed solid and liquid media compressed to the size of the order of the one wavelength of hard ultraviolet or soft X-ray pulses of energy.[1]

Studying of energy storage in quantum nanoparticles is needed for the development of new femtosecond pulse processing techniques that do not destroy the functional and biomimetic materials. Quantum-sized nanoparticles of energy storage in common is that because of the small area of their localization processes of accumulation and dissipation of energy are determined by the laws of quantum kinetics with characteristic time intervals of quantum transitions from tens to a few hundredths of femtoseconds with the uncertainty of energy from 0.1 eV to 1 keV, respectively.[1] In this paper some properties of quantum NEMS accumulators of compressed pulses of energy such as nanobots are investigated. Simulated evolution of nanobot in fcc crystal of iron was held in the framework of quantum NEMS-kinetics (NK).[2] For comparison we present results of investigation of evolution the atomic cluster of iron having structure similar to the nanobot. The result was obtained by molecular dynamics (MD) method.[3]

2. The Theory of Quantum NEMS Accumulators of Energy Storage in the Condensed State

The nanobot is a movable compact quantum NEMS.[2] One can imagine that the nanobot include electron quantum motor and quantum mechanical moving part of nuclei. The nuclear quantum-mechanical moving part is driven by the electronic engine. The motor acts in a compact physical space domain V of the condensed state. It is a specific open subsystem of strongly correlated N_v electrons having form of compact electron quasiparticle (N_v-compacton) such as some electron compaction inside electronic environment of the condensed state.[4] The number N_v f electrons in the N_v-compacton fluctuates about basic values N_{v0} preserving the average number of electrons $\langle N_v \rangle = N_{v0}$ since general quantum states of the closed composite strong-correlated system "N_v-compacton + electronic environment of the condensed state" have the common entanglement form[2]:

$$\Phi(N_v^0; \infty - N_v^0) = C_{Nv0}\Psi(N_v^0)\Phi(\infty - N_v^0) + C_{Nv0\pm1} \times \Psi(N_v^0 \pm 1)\Phi(\infty - (N_v^0 \pm 1)) + \dots \quad (1)$$

where entangled coherent transfer of $n = 1, 2, \dots$ electron pairs N_v-compacton quantum states $\Psi(N_v^0 \pm n)$ and the quantum field of the electron component (environment) of the condensed state $\Phi(\infty - (N_v^0 \pm n))$, respectively:

$$\Psi(N_v^0 \pm n) = [\Psi(N_v^0 + n) + \Psi(N_v^0 - n)]/\sqrt{2} \quad (2)$$

$$\Phi(\infty - (N_v^0 \pm n)) = [\Phi(\infty - N_v^0 - n) + \Phi(\infty - N_v^0 + n)]/\sqrt{2}. \quad (3)$$

In quantum states of (1) the amplitudes are normalized to unity:

$$|C_{Nv0}|^2 + |C_{Nv0\pm1}|^2 + |C_{Nv0\pm2}|^2 + \cdots + |C_{Nv0\pm n}|^2 + \cdots = 1. \quad (4)$$

Spontaneous breaking of dynamical symmetry of quantum field of the electron component of the condensed state in the V-domain is described in the limit of $1 \approx C_{Nv0} \gg C_{Nv0\pm1} \approx 0$, when there is an open electronic N_v-compacton in the "zero" state $\Phi_0(N_v^0)$:

$$\Phi_0(N_v^0) = C_{Nv0}\Psi(N_v^0)\Phi(\infty - N_v^0) + C_{Nv0\pm1}\Psi(N_v^0 \pm 1)\Phi(\infty - (N_v^0 \pm 1)). \quad (5)$$

The original "zero" state $\Phi_0(N_v^0)$ is described in the quantum field theory by Fock subspace with the number of electrons $N_v = N_v^0$; $N_v^0 \pm 1$.

Then, using (5), Eq. (1) becomes:

$$\Phi(N_v^0; \infty - N_v^0) = \Phi_0(N_v^0) + \Phi_1(N_v^0). \quad (6)$$

Correction $\Phi_1(N_v^0)$ to "zero" state $\Phi_0(N_v^0)$ allows for an orderly transfer of charge and spin between the N_v-compacton and the electronic component of the condensed state of two or more electron pairs:

$$\Phi_1(N_v^0) = C_{Nv0\pm2}\Psi(N_v^0 \pm 2)\Phi(\infty - (N_v^0 \pm 2)) + \cdots + C_{Nv0\pm n}\Psi(N_v^0 \pm n)\Phi(\infty - (N_v^0 \pm n)). \quad (7)$$

The quantum nanobot NEMS is created, when the electronic N_v-compacton captures B nuclei subsystem in the V-domain of the condensed state. A quantum state $\Psi_0(B; N_v^0)$ incoherent association quantum-mechanical subsystem B nuclei and the

Nv-compacton of electrons has multiplicative quantum state vector $\Psi_0(\mathrm{B}\,|\,\mathrm{N}_\mathrm{v}^0)$:

$$\Psi_0(\mathrm{B}\,|\,\mathrm{N}_\mathrm{v}^0) = \chi_0(\mathrm{B})\Phi_0(\mathrm{N}_\mathrm{v}^0). \tag{8}$$

Taking into account (6) a tangled coherent state Ψ_1 $(\mathrm{B}\,|\,\mathrm{N}_\mathrm{v}^0)$ combined system $\mathrm{N_v}$-compacton of electrons and B nuclei becomes:

$$\Psi_1(\mathrm{B}\,|\,\mathrm{N}_\mathrm{v}^0) = \chi_0(\mathrm{B})\Phi_0(\mathrm{N}_\mathrm{v}^0) + \chi_1(\mathrm{B})\Phi_1(\mathrm{N}_\mathrm{v}^0), \tag{9}$$

where $\chi_1(\mathrm{B})$ is a correction to the wave function $\chi_0(\mathrm{B})$ of B nuclei, which takes into account a coherent entanglement the nuclear motion with multi-pair charge polarization of $\mathrm{N_v}$-compacton having the form (7).

The physical meaning of the Eqs. (8) and (9) consists in that they represent the two quantum mechanical mechanism of electronic driving nuclear mechanical part NEMS. Equation (8) corresponds to the mechanism of incoherent untangled electronic driving nuclear mechanical part of the quantum nanobot. Equation (9) describes the mechanism of coherent moving nuclear subsystem tangled with the electronic component of the quantum NEMS.

Potential energy $\varepsilon_0(\mathrm{R})$ electronic drive nanobot's nuclei depends on the kinematics of electronic bonds tangling nuclei. There are three types (α, β, γ) kinematic constraints in the electronic drive nuclei.[5] Topology kinematics constraints are given graph $\mathrm{G}_{\alpha\beta\gamma}$, whose vertices are the nuclei and edges are existing kinematic coupling between the nuclei of one of three types — α, β, γ.

Figure 1 shows a graph $\mathrm{G}_{\alpha\beta\gamma}$ for a specific system of three nanobots containing $\mathrm{B} = 6$ nuclei.[5]

Figure 1 shows that the (α, β, γ) electronic kinematic constraints nuclei differ in their belonging of spatial media: internal kinematic α-constraints wholly owned V-region of only one electronic compacton (nanobot), transboundary β-constraints — two or more compactons overlapping areas V, and

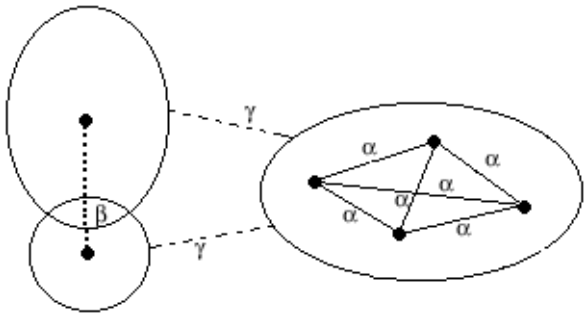


Fig. 1. Topological graph $\mathrm{G}_{\alpha\beta\gamma}$ electronic kinematic constraints nuclei three nanobots.

external γ-connection — the contact area of compacton with the condensed state matrix.

For given graph $\mathrm{G}_{\alpha\beta\gamma}$ kinematic constraints B nuclei the energy of nanobots can be written as:

$$\varepsilon_0(\mathrm{R}) = \varepsilon_0(\mathrm{R}\,|\,\Gamma_{\alpha\beta\gamma}) = (1/2)\sum_{\mathrm{p}}\sum_{\mathrm{p}'} S^k_{\mathrm{pp}'}\varepsilon^k_{\mathrm{pp}'}(\mathrm{R}_{\mathrm{pp}'}). \tag{10}$$

Here $\mathrm{p} = 1, \ldots, \mathrm{B}$, $p' = 1, \ldots, \mathrm{B}$ — indices nuclei nanobots — vertices of graph $\mathrm{G}_{\alpha\beta\gamma}$; $(\mathrm{S}^k_{\mathrm{pp}'})$ — k-matrix $(\mathrm{k} = \alpha,\ \beta,\ \gamma)$ attached wires — edges of graph $\mathrm{G}_{\alpha\beta\gamma}$; $(\varepsilon^{\mathrm{k}}_{\mathrm{pp}'}(\mathrm{R}_{\mathrm{pp}'}))$ — k-matrix $(\mathrm{k} = \alpha,\ \beta,\ \gamma)$ energy ties p and p′ nuclei, $\mathrm{R}_{\mathrm{pp}'}$ — internuclear distance at the point of the configuration space R of B nuclei. The method of nonlocal density functional that explicitly depends on the type of α-, β-, γ-ties is used for calculation the energy matrix k-ties $(\varepsilon^{\mathrm{k}}_{\mathrm{pp}'}(\mathrm{R}_{\mathrm{pp}'}))$.[4–6]

Quantum relaxation kinetics nanobot is a chain of discrete stages alternating mechanisms of action of two coherent and incoherent electronic drive motion of the nuclear subsystem NEMS. Changing the electronic drive mechanism described by the theory of nuclei NEMS processes "coherence-decoherence" motion of quantum systems.[7]

Thermal motion of the matrix of the condensed state limits the duration τ of step coherent electronic drive nuclei nanobot[8]:

$$\tau = \{[3\mathrm{BkT}]/[(\mathbf{grad}_{\mathbf{R}_0}\varepsilon_0)\mathbf{M}^{-1}(\mathbf{grad}_{\mathbf{R}_0}\varepsilon_0)]\}^{1/2}, \tag{11}$$

where T — temperature of the condensed state, B — number of the nuclei, M^{-1} — the inverse tensor of the mass distribution of the nuclei, and $\mathbf{grad}_{\mathbf{R}_0}\varepsilon_0$ — gradient energy $\varepsilon_0(\mathrm{R}\,|\,\mathrm{G}_{\alpha\beta\gamma})$ electronic drive nuclei in the vicinity of the configuration point R.

For small nanobots and low temperatures from (11) it follows that the stages of coherent electronic drive nuclei have femtosecond duration, which is one–two orders of magnitude less than the oscillation period of the atoms in the matrix of the condensed state. As a result of thermal failure of coherence there is a reduction of the coherent state of nanobots (9) in an incoherent state (8):

$$\chi_0(\mathrm{B})\Phi_0(\mathrm{N}_\mathrm{v}^0) + \chi_1(\mathrm{B})\Phi_1(\mathrm{N}_\mathrm{v}^0) \Rightarrow \chi_0(\mathrm{B})\Phi_0(\mathrm{N}_\mathrm{v}^0). \tag{12}$$

Recovering quantum coherence occurs during $\delta\tau \sim 0.01$ fs.

3. Simulation of Quantum Relaxation NEMS Energy Storage Cuboid Bots in the FCC Iron

In computer simulations the initial saturation energy of the investigated NEMS energy storage cuboid bots is modeled by fixing their original crystalline atomic clusters in the crystal facet planes (100) and subsequent replacement of the interatomic potentials in the crystalline atomic clusters on pseudopotentials internuclear α-constraints that operate inside the bot (α-bond) and at its boundary with the rest of the crystal matrix (external γ-bonds) as shown in Fig. 2.

Let us take under consideration a relaxation at normal temperature $T = 293\,K$ bounded by planes (100) cuboid nanobot Fe_{172} in the fcc lattice of iron. Energy stored in the iron crystal nanobot's cuboid is calculated from the formula (10). According to the calculation method of the nonlocal density functional energy α-bonds within the NEMS cuboid nanobot are much greater than the energy of the external Van der Waals γ-bonds the NEMS cuboid nanobot with a matrix of iron. Therefore relaxation performed neglecting γ-bonds with the matrix metal.

Figure 3 shows a diagram of the relaxation in the coordinates "energy per atom versus time". It can be seen that the kinetic energy loss curve the NEMS cuboid nanobot drive fluctuates. Thus there are two structural transformations on 20 and 40 picoseconds. The first corresponds to the appearance of characteristic "hyperboloid" bends faces, and the second — "trapezoid" deformation faces shown in Fig. 3(a).

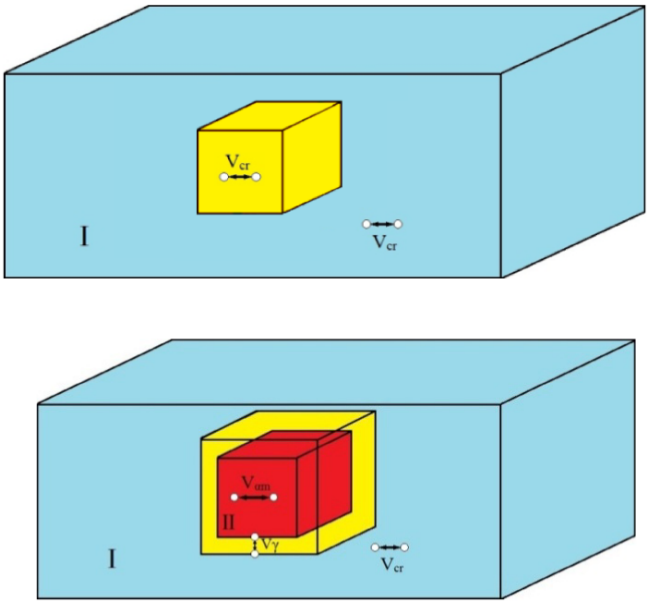
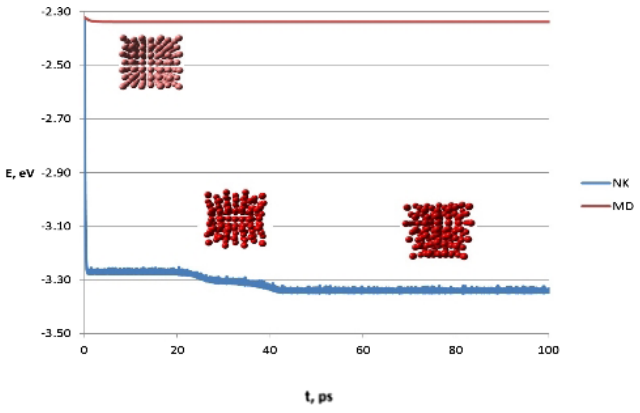
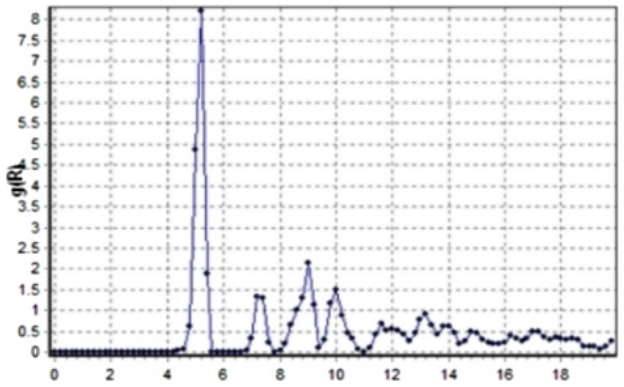


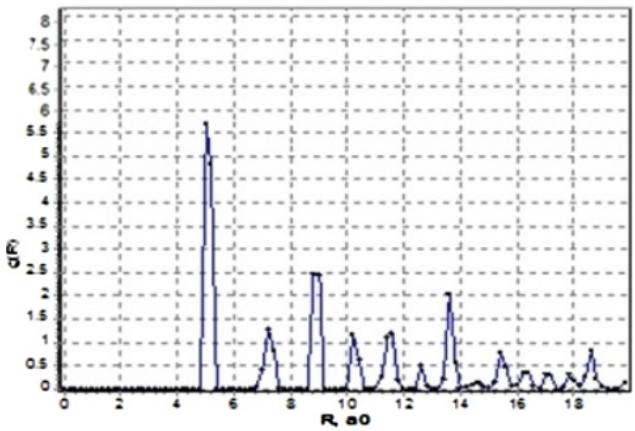
Fig. 2. NEMS energy storage cuboid bot (II) and its atomic cluster in the crystalline matrix (I). V_{cr} — potentials of interatomic bonds in the crystal matrix and within the cluster, V_α — pseudopotentials internuclear kinematic α-bonds in the nanobot, V_γ — pseudopotentials kinematic γ-bonds between the nanobot and crystal matrix.



(a)



(b)



(c)

Fig. 3. (a) Kinetics: NEMS nanobot (NK), atomic cluster (MD). (b) Pair radial distribution function of the nuclei g(r) the NEMS nanobot. (c) The atomic cluster after relaxation.

During relaxation the NEMS energy storage cuboid nanobot the pair radial distribution function of the nuclei g(r) are substantially modified [Fig. 3(b)]. It is growing short-range order due to the increase of the peak height on the first coordination sphere and the long-range order is destroyed by erosion of the peaks in the third and subsequent coordination spheres. During the relaxation function g(r) varies greatly and binding energy of the NEMS bot significantly by 1.01 eV/atom increases, reaching a value of 3.34 eV/atom in a relaxed state. This energy is only 1 eV/atom lower binding energy in the fcc iron crystal.

For comparison, Fig. 3 shows obtained by molecular dynamics[7] the results of calculation of relaxation at a temperature T = 293 K the iron atom cluster Fe_{172} in the absence of a spontaneous transition to the quantum state NEMS energy storage cuboid Fe_{172} nanobot. In the simulation we used the optimized fit to the experimental parameters of interatomic interaction in fcc iron crystal Morse potentials. Excess energy cluster in the method a molecular dynamics with respect to the fcc crystal is completely determined by the pair radial distribution function g(r) atoms [Fig. 3(c)]. With an increasing number of atoms in the cluster, the radial function g(r) and the binding energy per atom approaching values in the infinite fcc iron crystal bulk.

Figure 3(a) shows that the relaxation of the cluster iron in the molecular dynamics method is negligible. During the relaxation function g(r) [Fig. 3(c)] changes little, and the cluster lowers the energy by 0.02 eV/atom, achieving energy 2.34 eV/atom, which is about 2 eV/atom lower than the binding energy of the binding energy of the bulk crystal (4.30 eV/am).

From a comparison of g(r) in Figs. 3(b) and 3(c) it can be seen at the expense of what relaxation NEMS nanobot is a significant increase in the binding energy. This is a result of changes in short-range self-organization by increasing the effective coordination number from 5.5 to 8 in the first coordination sphere and the destruction of long-range order in the third and higher coordination spheres.

4. Conclusions

According to the quantum theory of the structure considered NEMS energy storage nanobots in materials in their modeling can be divided into two stages. At the first stage the atomic cluster in the crystal is formed by a sudden break ties with the crystal matrix on the boundaries of its spatial carrier. Furthermore there is a spontaneous breaking of dynamical symmetry of the electron component of the atomic cluster with the formation of electron compacton performing drive nuclei in the NEMS energy storage nanobot. In this rearranged crystalline interatomic chemical bonds in internuclear kinematic constraints NEMS of three types: internal (α), transboundary (β), external (γ) bonds, and molecular dynamics atomic cluster passes in quantum NEMS relaxation kinetics.

Within the simulation of NK-method the relaxation NEMS energy storage in the form of limited planes (100) Fe_{172} cuboid in fcc iron crystal was studied. It is spotted an opportunity to undergo a process of self-organization the NEMS energy storage cuboid nanobot through several intermediate metastable states. It is shown that in the region of several tens of picoseconds in the relaxation process fluctuation rebuild the cube cuboid occurs with a strong bending of the surface edges, and then their transformation in the "trapezoid". This differentiates NK relaxation NEMS energy storage Fe_{172} nanobot from MD relaxation Fe_{172} clusters of atoms in crystalline iron.

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