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STRUCTURE AND PROPERTIES OF NANOSCALE AND MESOSCOPIC MATERIALS

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Nickel Nanowires Based on Icosahedral Structure

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One-dimensional atomic systems modelling nickel nanowires are constructed on the base of icosahedral structural motif. The structure evolution of icosahedral nanoparticles and nanowires with temperature is examined by molecular dynamics simulations as a function of their shape and size. The drastic change of regular solid shape (shape transformation) detected in Ni icosahedral nanowires is interpreted as a specific type of solid state transformation in one-dimensional system that is controlled by surface diffusion.

Key words: nanowire, nanoparticle, icosahedron, one-dimensional system, melting temperature, Rayleigh instability, surface diffusion.

Одновимірні атомні системи, які моделюють нікелеві нанодроти, були побудовані на основі ікосаедричного структурного мотиву. Вплив температури на еволюцію структури в ікосаедричних наночастинках і нанодротах був досліджений методом молекулярної динаміки як функція їх форми та розмірів. Радикальна перебудова форми твердого тіла (перетворення форми), виявлена в Ni ікосаедричних нанодротах, була трактована як специфічний тип твердотільного перетворення в одновимірній системі, який контролюється поверхневою дифузією.

Ключові слова: нанодріт, наночастинка, ікосаедр, одновимірна система, температура плавлення, Релеєвська нестабільність, поверхнева дифузія.

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Одномерные атомные системы, которые моделируют никелевые нанопроволоки, были построены на основе икосаэдрического структурного мотива. Влияние температуры на эволюцию структуры в икосаэдрических наночастицах и нанопроволоках было исследовано методом молекулярной динамики как функция их формы и размеров. Радикальное перестроение формы твёрдого тела (превращение формы), выявленное в Ni икосаэдрических нанопроволоках, было трактовано как специфический тип твердотельного превращения в одномерной системе, которое контролируется поверхностной диффузией.

Ключевые слова: нанопроволока, наночастица, икосаэдр, одномерная система, температура плавления, Рэлеевская нестабильность, поверхностная диффузия.

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1. INTRODUCTION

The magnetic nanowires present a special class of one-dimensional materials that have the form of a wire with a radial size falling in the range of 1–100 nm. The high surface-to-volume ratio of nanowires provides a lot of useful properties and enables its promising applications in nanoscale electronics, phase-change memory, $3D$ magnetic memory, magneto-sensors, permanent magnets, magnetic refrigerators, magnetic hyperthermia, biomedical drug-delivery systems, chemical catalysts [1–8].

As the heating processes are often involved in preparation and functioning of nanoscale devices, the ability to predict the influence of size and shape on morphological stability and melting temperature of nanoparticles and nanowires is of great importance. Size dependent depression of melting temperature and phenomenon of Rayleigh instability are the main causes of thermal break of nanoscale structures.

The melting temperature of nanoparticles with different sizes and shapes was investigated by means of experiments and molecular dynamic simulations [9–15]. The inverse proportionality between depression of melting temperature and the size of rounded particles was found, and the smaller the size of particle, the greater the effect of shape.

The Rayleigh instability is supposed to be responsible for the thermally induced morphological transformation observed in annealed nanowires [16–20]. At this transformation cylindrical nanowires decompose on a periodic succession of spherical nanoparticles with the same diameter, which depends on the radius of initial nanowire. The transformation is controlled by surface diffusion of atoms along the wire from the neck regions towards the convex ones due to Laplace pressure deviations obeyed by surface curvature.

In this paper, we develop the models of nickel icosahedral nanowires and study the effect of particle shape and size on its thermal stability.

2. METHODS OF ATOMISTIC SIMULATIONS

Molecular Dynamics (MD) simulations were carried out with the open source XMD program [21]. Atomic interactions are modeled using the embedded atom method (EAM) [22]. The total energy of N atom system is given by

$$U=\sum_{i=1}^{N}F_i(\rho_i)+\sum_{i=1}^{N}\sum_{i>j}^{N}\varphi_{ij}(r_{ij});\ \rho_i=\sum_{i\neq j}f_i(r_{ij}),$$

where the embedding energy of i atom $F_i(\rho_i)$ is a function of local electron density ρ_i contributed by each of the neighbouring atoms j at position r_i, and $\varphi_{ij}(r_{ij})$ is a pairwise interaction potential between the current atom i and neighbouring atom j, which depends only on the interatomic separation distance r_{ij}. The functions F, f, φ for Ni were defined from [23].

The systems were treated as NPT ensembles. The temperature was changed by rescaling atomic velocities. Constant pressure $p = 0$ Pa was kept by system volume adjustment.

The simulations were carried out with the time step $1\cdot10^{-15}$ s and the atomic velocity rescaling every 200 steps. Heating (cooling) of systems was performed at the heating (cooling) rate $2\cdot10^{10}$ K/c.

The temperatures of structural transitions were identified with the leaps on temperature dependence of potential energy. At tensile mechanical testing of nanowires, the coordinates of one nanowire side were fixed and another side was forced along five-fold symmetry axis.

Simulation results were visualized with the OVITO software [24].

3. RESULTS AND DISCUSSION

Two-stage approach has been applied to construct the models of Ni nanorods and nanowires based on icosahedral structural motif. At the first stage, three small Ni clusters with 15, 55, and 147 (magic numbers) atoms were cut from the ideal face-centred cubic structure. Using molecular dynamics simulation, the f.c.c. clusters were heated for melting and then cooled to low temperature. After cooling we received the set of highly symmetric 13, 55, and 147-atomic particles (Fig. 1) in equilibrium shape with icosahedral structure. The size of particles is equal to 0.472, 0.948, and 1.424 nm, and potential energy at 1 K equals to −3.46, −3.83, and −3.99 (eV/at) for 13, 55, and 147-atomic particles, respectively. Thereafter these particles were used for construction of nanorod and nanowire models.

The icosahedral structure (Ih) is resulted from packing together twenty elastic distorted f.c.c. tetrahedrons, that are in {111} twin-related conjunctions and share a common vertex. The Ih cluster has 20 (111)-like facets, 30 edges, 6 five-fold symmetry axes, and 15 symmetry planes. Examples of (111) facet and five-fold symmetry axis are designated by colour on Fig. 1 for 13, 55, and 147-atomic particles. The plane, that is normal to five-fold symmetry axis and crosses Ih centre (layers 3, 5, 7 on Figs. 1, *c*, *g*, *k*), divides the icosahedron on two parts and becomes a mirror plane after $\pi/5$ rotation either of these icosahedron parts around the five-fold symmetry axis.

Consider as an example the construction of nanorod and nanowire on the base of 55-atomic Ih cluster that is composed of nine atomic layers (Nos. 1–9 on Fig. 1, *g*) normal to selected five-fold symmetry axis. Af-

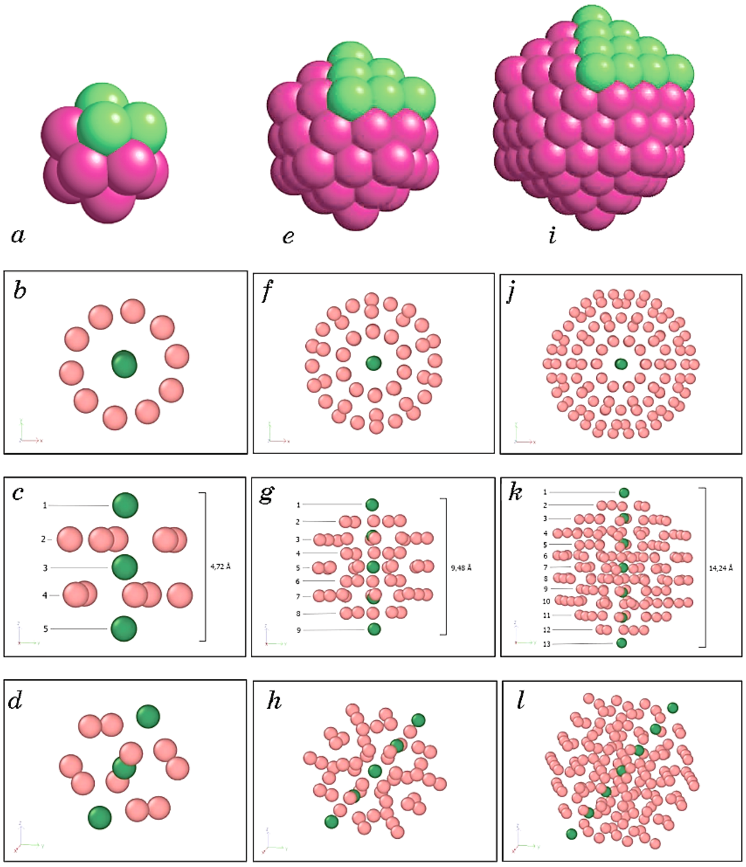

Fig. 1. The shape and structure of 13 (*a*–*d*), 55 (*e*–*h*), and 147-atomic (*i*–*l*) Ni icosahedral particles.

ter deletion of atomic layer No. 9 of initial cluster, the copies of cluster layers Nos. 1–5 were added to the cluster in back order, being renamed into numbers Nos. 9–13. The result of layers stacking is a 13-layered nanorod (Fig. 2).

By reiteration of stacking operation, the NW13, NW55, and NW147 nanowires (based on 13, 55, and 147-atomic Ih clusters, respectively) were constructed with length-to-diameter ratio equal to 20 (Fig. 3). At this ratio the thermodynamic and mechanical properties of nanowires become independent on length. The structures of end vertexes and the diameters of nanowires (equal to 0.472, 0.948, and 1.424 nm) are the same as that of initial 13, 55, and 147-atomic icosahedra.

Structure evolution of Ih nanoparticles and nanowires with temperature was examined as a function of their shape and size in heating-cooling thermal cycle. For Ih nanoparticles, on heating branch of thermal cycle up to melting point, the temperature dependence of potential energy is linear and no changes in shape and atomic structure are observed (Fig. 4, *a*–*c*). Melting temperature equals to 850, 950, and 1150 K for 13Ih-, 55Ih-, and 147Ih-particles and decreases with a decrease of particle size. Hysteresis loop on temperature dependences of potential energy for 55Ih- and 147Ih-particles is caused by undercooling of liquid phase on back branch of thermal cycle.

On the contrary to Ih nanoparticles, the temperature evolution of

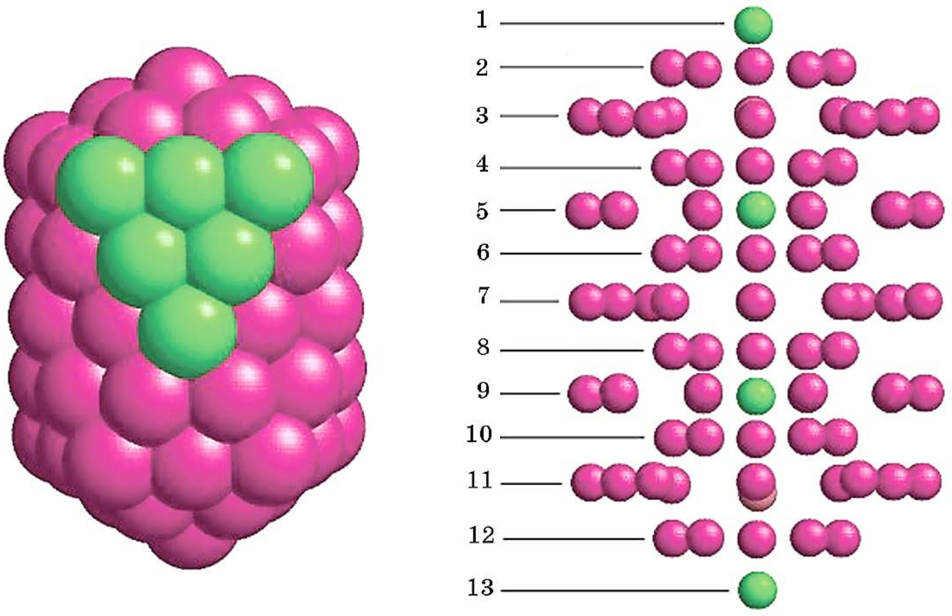

Fig. 2. The shape and Ih structure of 13-layered nanorod based on 55-atomic Ni icosahedron.

shape and structure of nanowires is more complicated. The nanowires reveal a morphological transformation foregoing the nanowire melting. The temperature of shape transformation was measured at abrupt decrease on temperature dependence of potential energy and equals to 710 K, 910 K, and 1150 K for NW13, NW55, and NW147 nanowires, respectively (Fig. 4, *d–f*).

The shape transformation begins at the ends of nanowire with appearance of ending bulbs and completes with formation of rounded particle generally composed of two decahedrons (Fig. 5).

After completion of shape transformation this faceted solid state particle (Fig. 5, *d*) continues heating until melting (Fig. 5, *e*). The melting temperatures are equal to 1150 K, 1300 K, and 1500 K for NW13, NW55, and NW147 nanowires, respectively (Fig. 4, *d–f*).

It is worth to note the essential feature of studied nanowires, namely, a great fraction of surface atoms (0.83, 0.62, and 0.49 for NW13, NW55, and NW147 nanowires, respectively). For this reason the shape transformation in nanowires, defined as a drastic change of regular solid shape without melting, can be supposed to be a specific type of solid state transformation in one-dimensional nanosystems that is controlled by surface diffusion.

Elastic modulus, tensile strength and fracture behaviour of nan-

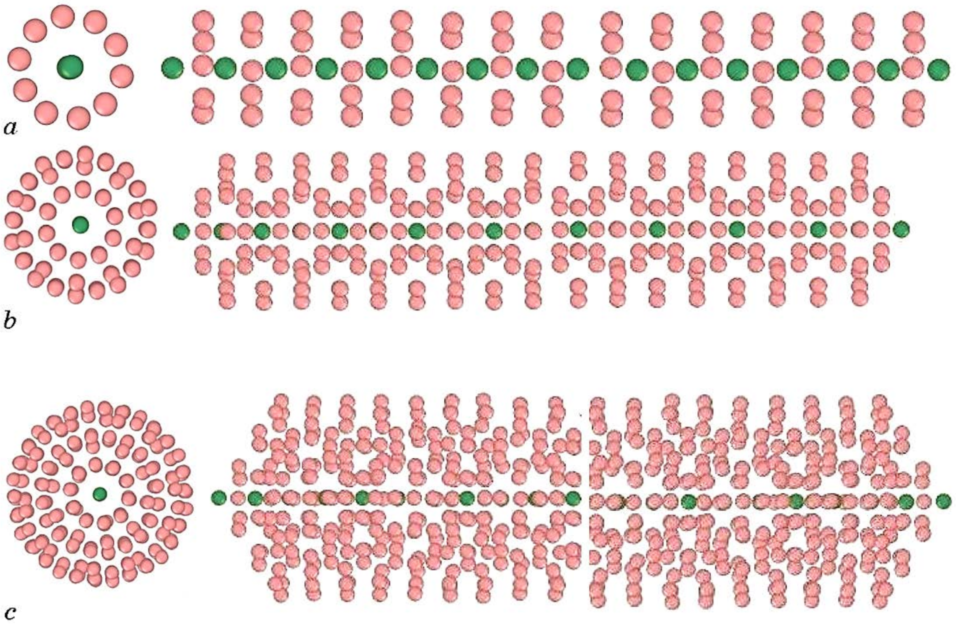

Fig. 3. The structures of NW13 (*a*), NW55 (*b*), and NW147 (*c*) nanowires based on 13, 55, and 147-atomic Ni icosahedra.

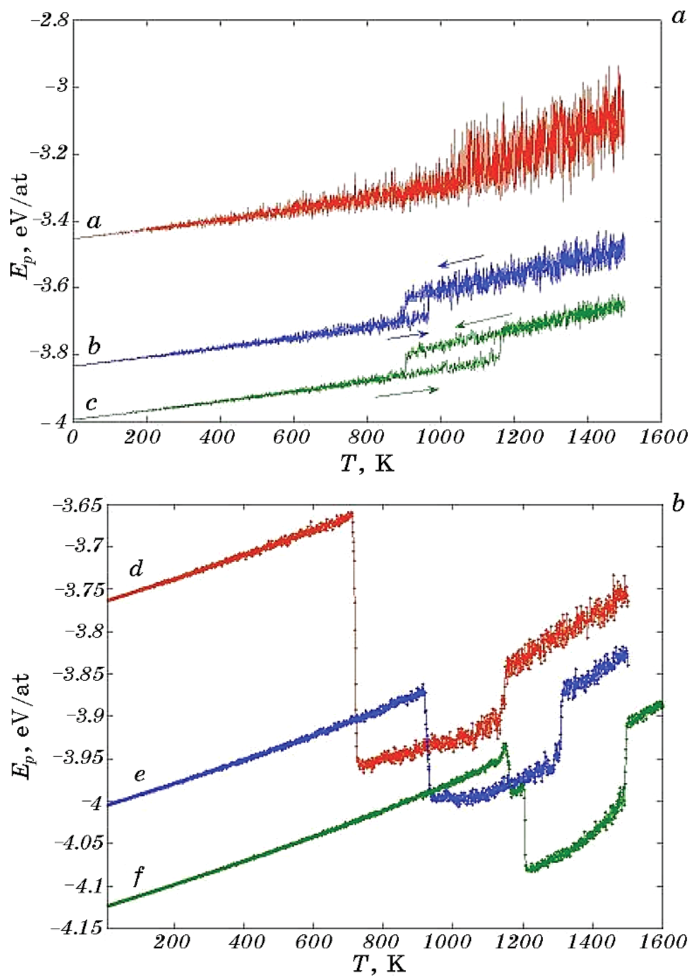

Fig. 4. Temperature dependence of potential energy of nanoparticles (13 at. Ih (*a*), 55 at. Ih (*b*), 147 at. Ih (*c*)) and nanowires (NW13 (*d*), NW55 (*e*), NW147 (*f*)).

owires are dependent on diameter (Table 1, Fig. 6).

The fracture of NW13 nanowire is a brittle-like detachment. The NW55 and NW147 nanowires exhibit a significant viscous flow with neck formation.

4. CONCLUSIONS

The models of nickel nanowires were constructed on the base of icosahedral structural motif.

The structure evolution in icosahedral nanoparticles and nanowires with temperature was examined as a function of their shape and size.

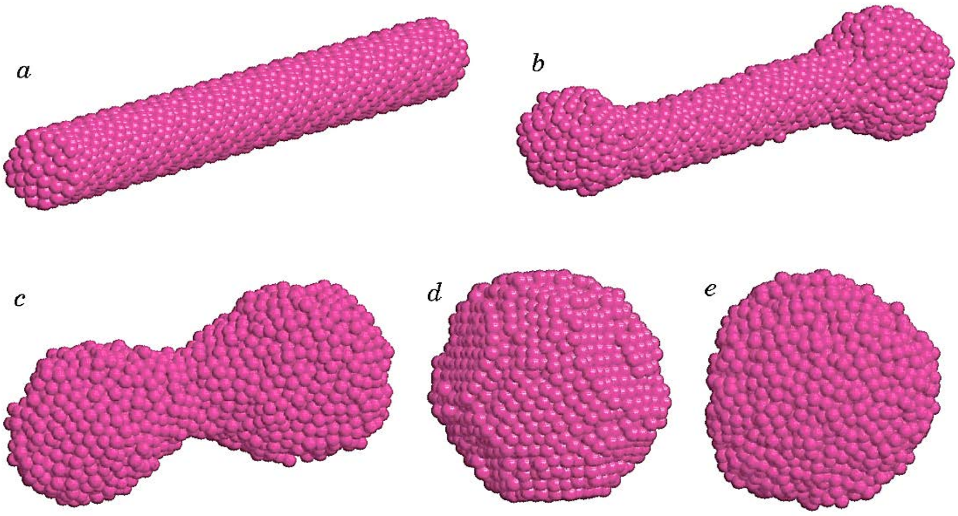

Fig. 5. Shape and structure evolution of NW147 nanowire with temperature on heating branch of thermal cycle (1 K (*a*), 1150 K (*b*), 1160 K (*c*), 1220 K (*d*), 1600 K (*e*)).

TABLE 1. Elastic modulus and tensile strength of nanowires tested at 300 K.

Test	NW13	NW55	NW147
E (GPa)	180	230	270
σ (GPa)	13.7	10.9	11.1

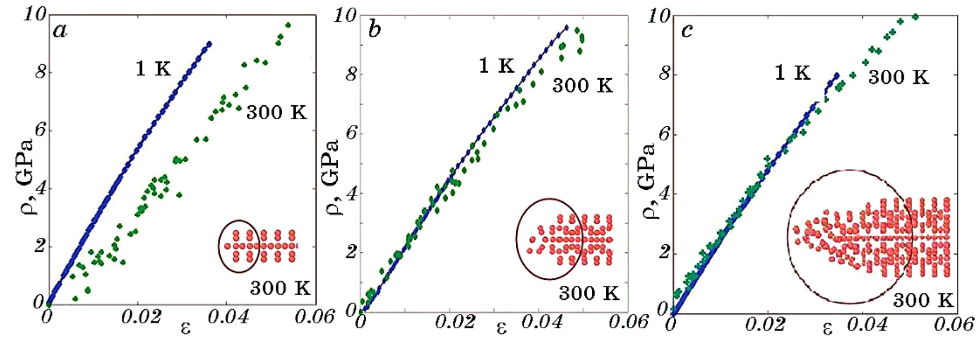

Fig. 6. Stress-strain curves and fracture of NW13 (*a*), NW55 (*b*), and NW147 (*c*) nanowires tested at temperatures 1 K and 300 K.

The morphological transformation (shape transformation) was detected in Ni icosahedral nanowires.

This shape transformation in nanowires, defined as a drastic change of regular solid shape without melting, can be referred to specific type of solid state transformations in one-dimensional nanosystems that are controlled by surface diffusion.

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