Original paper

Dynamics of thermally induced structural transformations in a ternary $Pd_4@Ni_2@Pt_2$ nanocube

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Abstract: Using isothermal molecular dynamics and LAMMPS software, we studied the dynamics of chemical and structural segregation upon heating $Pd_4@Ni_2@Pt_2$ nanocubes from 300 to 2000 K (the subscripts indicate the number of atomic monolayers). The embedded atom method was used for simulations. The system was preliminarily subjected to relaxation for 1 ns at a temperature of 300 K. Particular attention was paid to analyzing the temperature dependence of the specific potential energy and its relationship with structural transformations at temperatures near which some jumps in this dependence occur. Several types of transitions were identified: fcc/hcp structural transitions, order/disorder transitions associated with competition between identified and unidentified crystalline phases, sphere-to-polyhedron and vice versa transitions corresponding to shape changes, and a complex melting phase transition with an atypical behavior of the temperature dependence of the specific potential energy. Two alternative approaches were used for the first time to identify the local environment: the polyhedral template method and the Ackland-Jones method. The identification results using both methods are generally in good agreement, but the Ackland-Jones method sometimes identifies as bcc instead of the hcp local environment (when the polyhedral template method was employed), and this seems apparently be due to a feature of the Ackland-Jones method based on an analysis of the distribution of bond angles between the central atom and its nearest neighbors.

Keywords: nanocube $Pd_4@Ni_2@Pt_2$, Ackland-Jones method, polyhedral template matching, LAMMPS, molecular dynamics, embedded atom potential, structure transformations.

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Динамика термоиндуцированных структурных превращений в тернарном нанокубе $Pd_4@Ni_2@Pt_2$

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Аннотация: С использованием изотермической молекулярной динамики и ПО LAMMPS проведено исследование динамики химической и структурной сегрегации при нагреве

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нанокубов $Pd_4@Ni_2@Pt_2$ от 300 до 2000 К (нижние индексы отвечают числу атомных монослоев). Для моделирования использовался метод погруженного атома. Предварительно система подвергалась релаксации в течение 1 нс при температуре 300 К. Особое внимание уделено анализу температурной зависимости удельной потенциальной энергии и ее взаимосвязи со структурными превращениями при температурах, в окрестности которых имеют место скачки на этой зависимости. Идентифицировано несколько типов переходов: структурные переходы типа ГЦК/ГПУ, переходы типа порядок/беспорядок, связанные с конкуренцией между идентифицированными и не идентифицированными кристаллическими фазами, переходы сфера-многогранник и наоборот, отвечающие изменению формы, а также фазовый переход плавления сложного типа с нехарактерным поведением температурной зависимости удельной потенциальной энергии. Для идентификации локального окружения впервые использовались два альтернативных подхода: метод полиэдральных шаблонов и метод Экленда-Джонса. Результаты идентификация при использовании обоих методов в целом находятся в хорошем согласии, но метод Экленда-Джонса иногда идентифицирует ОЦК-вместо ГПУ-локального окружения (метод полиэдральных шаблонов), что, по-видимому, связано с особенностью метода Экленда-Джонса, который основан на анализе распределения углов связей между центральным атомом и его ближайшими соседями.
Ключевые слова: молекулярная динамика, LAMMPS, метод погруженного атома, нанокуб $Pd_4@Ni_2@Pt_2$, метод Экленда-Джонса, метод полиэдральных шаблонов, структурные превращения.

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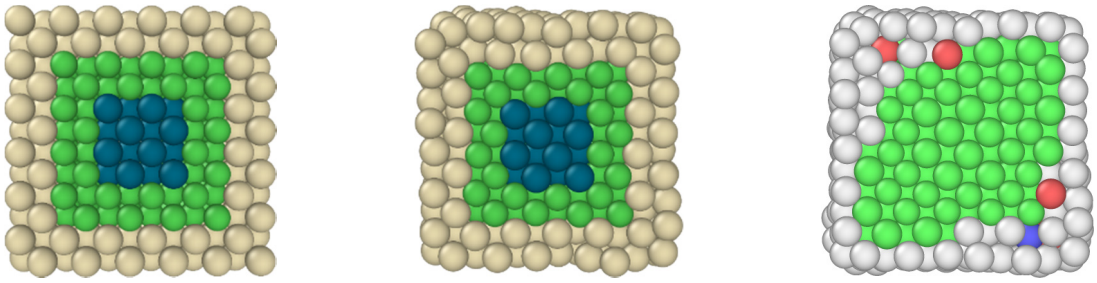
1. Introduction and statement of the problem

As a rule, works on atomistic modeling of metallic nanosystems are devoted to investigations of objects with the simplest spherical morphology for both mono- and multicomponent metallic nanoparticles [1-4]. At the same time, the study of morphologies other than spherical allows, no doubt, to expand the areas of application of multicomponent nanoparticles. Thus, one of the promising morphologies from a practical point of view are nanocubes containing several shells [5-7]. For example, in [7], $Pd@Ni@Pt$ nanocubes were synthesized and their catalytic properties were studied. This work served as an incentive for conducting our research using isothermal molecular dynamics to analyze thermally induced transformations in ternary $Pd@Ni@Pt$ nanocubes. Earlier [8], using the tight-binding potential in $Pd_4@Ni_2@Pt_2$ nanoparticles (the subscripts indicate the number of shells in the layer), we identified for the first

time a structural transition preceding their melting, which can be considered as the most interesting result of this work. However, a number of open questions remain, and one such question is the validation of the results using alternative software and alternative force fields for atomistic simulation. From a methodological perspective, this problem is consistently considered in a number of our studies [9-11].

In this work, to study the dynamics of thermally induced structural transformations in the ternary nanocube $Pd_4@Ni_2@Pt_2$ (the initial configuration is shown in fig. 1 a), we used the LAMMPS software [12], implementing isothermal molecular dynamics, and then the Ovito software [13], which allows us to identify the local structure of nanoparticles. In order to compare the results of the MD experiments with the data of [8], the temperature range from 300 to 2000 K was chosen, the heating rate was 0,3 K/ps, and the relaxation (annealing) time was 1 ns at a temperature of 300 K (the final configuration after relaxation is shown in fig. 1 b). The embedded atom potential with the parameterization [14] was used as the interatomic interaction method.



a b c

Fig. 1. Cross-section of the ternary system $Pd_4@Ni_2@Pt_2$ (a total of 864 atoms, including 608 Pt atoms, 224 Ni atoms, 32 Pd atoms): a – before and b – after relaxation for 1 ns. Visualization was performed in the Ovito software [13]: blue color – Pd atoms, green color – Ni atoms, beige color – Pt atoms, respectively. Panel c – local structure after relaxation. The local environment is designated as follows: green atoms – fcc local environment, red atoms – hcp, blue atoms – bcc, those unrecognized by the Ovito program [13] are designated in gray.

2. Simulation results and discussion

Caloric curves, i.e., the dependence of the specific potential energy of a nanoparticle on temperature, are one of the main tools for identifying phase (occurring with an increase in specific energy upon heating) and structural transitions (accordingly, occurring with a decrease in specific energy upon heating) [1]. Fig. 2 shows this dependence for the ternary system $Pd_4@Ni_2@Pt_2$ in the selected temperature range and indicates the characteristic temperatures corresponding to structural transitions (605, 843, and 1080 K) and melting (as will be shown below, the onset of melting corresponds to a temperature of 1283 K). In addition, red asterisks indicate sections of the caloric curve that are also of interest from the point of view of identifying structural transformations.

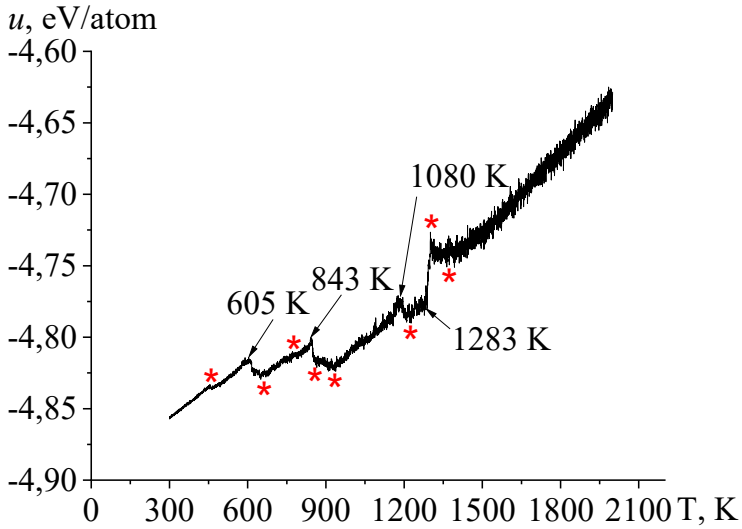


Fig. 2. Temperature dependence of the potential part of the specific internal energy of the ternary system $Pd_4@Ni_2@Pt_2$.

The analysis of the caloric curve shown in fig. 2 allows us to conclude that for the ternary three-shell system $Pd_4@Ni_2@Pt_2$, the phase transition corresponding to melting occurs in a quite narrow temperature range (from 1283 to 1301 K) that is not typical for binary and multicomponent metallic nanoparticles [1, 4], including ternary $Pd-Ni-Pt$ nanoparticles of a different initial morphology [9, 10]. In addition, on the caloric curve, the phase transition corresponding to melting has two sections: the pre-melting phase, but with almost complete destruction of the crystalline ordering (from 1200 to 1283 K) and melting in the classical interpretation of the caloric curve behavior (from 1283 to 1301 K), where the destruction of the crystalline structure is supplemented by sharply occurring segregation processes associated with the complete destruction of the shells: the inner core of palladium and the second shell of nickel.

However, it should be noted that for the ternary system $Pd_4@Ni_2@Pt_2$, the analysis of other, less pronounced structural transitions is of even greater interest. Although three characteristic temperatures are marked in this figure, as will be shown below, a number of patterns of structural and chemical segregation can only be identified through a combined study of the behavior of the caloric curve and the identification of local crystalline and quasi-crystalline phases, for example, by the polyhedral template matching method [13, 15] (PTM with the RMSD parameter equal to 0,155), which, in the temperature range close to the melting point, has the advantage of a local structure identification algorithm compared to the nearest neighbor method [16, 17]. For additional verification of the results, the Ackland–Jones analysis (AJA) [18] was used, which is based on the analysis of the distribution of bond angles between the central atom and its nearest neighbors.

Fig. 3 shows the results of identifying the local environment of atoms in a

ternary $Pd_4@Ni_2@Pt_2$ nanoparticle at various stages of its evolution. At a temperature of 450 K, active displacement of platinum atoms occurs. The nanocube vertices become less pronounced, which leads to a loss of local crystallinity near the vertices up to the 2nd-4th monolayer, but the overall proportion of crystalline phases is approximately 49% with a dominant fcc motif (43%). At the same time, local pyramidal hcp zones and individual bcc defects (their total proportion is slightly above 0,2%) are formed on the inner surface (i.e., the nanoparticle surface after removal of unrecognized atoms). This structural transformation can be identified as a *local* fcc→hcp transition. At a temperature of 605 K the displacement of atoms leads to an increase in local hcp and bcc zones in the nanocube volume, which initiates its deformation and the transition of the nanocube into a nanopolyhedron (this will be visualized later). The proportion of crystalline phases in the core also decreases, and these defects are clearly visible. However, overall, the fcc motif remains the dominant pattern, accounting for 30%, while the hcp motif accounts for only 11%.

With a further increase in temperature to 655 K, the proportions of fcc and hcp phases change only slightly – to 28% and 14%, respectively. In this case, the behavior of the caloric curve is apparently related not to atomic migration, but to the migration of the local structure, the emergence of hcp symmetry in regions of deformation caused by thermal expansion. Both templates (AJA and PTM) identify the behavior of the fcc environment in virtually the same way, but some hcp atoms are identified as bcc when using the AJA template.

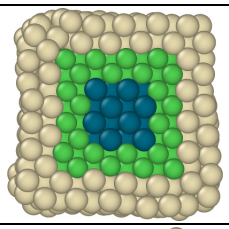
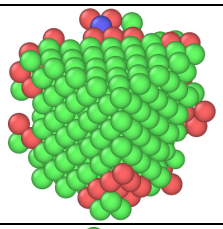
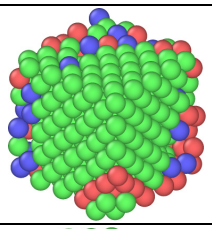
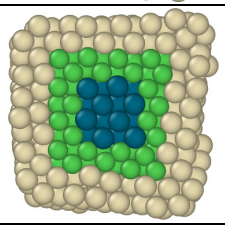
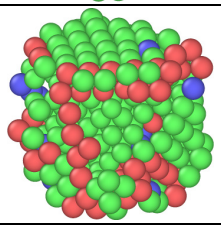
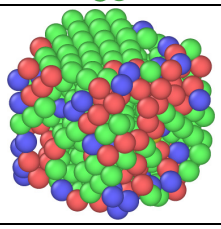
Of particular interest is the temperature of 776 K. At this temperature, the local structure in the second (relative to the outer one) atomic monolayer partially (not in all directions, but predominantly in one half of the nanoparticle) acquires greater order (fcc faces with hcp edges). It should also be noted that at this temperature, the proportion of the fcc phase is approximately 33% and exceeds the proportion of the hcp local environment (11%). The bcc phase also manifests itself as single defects. But the degree of crystallinity remains approximately at the same level of 48%.

At 843 K, a highly ordered structure with fcc faces and hcp edges has formed over the entire inner surface, and not in a single monolayer. Under the hcp layer are isolated bcc defects and a core of atoms not identified by the Ovito program [13]. The AJA modifier generally confirms the above-mentioned patterns, but identifies additional local bcc defects not only in the core but also on the inner surface of the nanoparticle. From a chemical segregation standpoint, the system remains relatively stable, experiencing only a wall deformation. This subsequently leads to the destruction of the crystallinity of the inner surface facets, which is readily identified by both modifiers. The AJA modifier, however, tends to identify the bcc phase. However, the PTM modifier's templates fail to recognize the surrounding environment as crystalline

ordered. Furthermore, the proportion of close-packed phases (fcc, hcp) continues to redistribute (not to decrease sharp!) to 24% and 16%, respectively. Upon reaching 850 K, a structural transition occurs associated with a change in the quasi-equilibrium shape: sphere → polyhedron. The proportion of crystalline phases is 39%. Thus, in this case, a structural transition occurs associated with a change in the quasi-equilibrium shape: sphere → polyhedron. The palladium core begins to disintegrate, and nickel atoms actively «break through» the inner (second) monolayers of platinum atoms. The ordering of the inner surface of the nanoparticle becomes more pronounced with a combination of fcc faces and hcp edges.

A temperature of 935 K can be considered the activation temperature for diffusion processes: nickel atoms begin to actively migrate to the surface, palladium atoms are located at the boundary between nickel and platinum atoms, and platinum atoms are just beginning to migrate into the core. Remarkably, the level of close-packed phases drops to 46%, and the proportions of close-packed phases (fcc, hcp) are 21 and 25%, respectively. A further increase in temperature to 1080 K maintains the faceting of the nanoparticle, but the degree of crystallinity begins to decrease, mainly due to defects in the core and on the inner surface of the nanoparticle at the intersection of the hcp edges.

As the temperature rises to 1200 K, nickel atoms emerge at the surface, platinum atoms are identified throughout the nanoparticle, and the palladium core is destroyed. The proportion of crystalline phases falls slightly below 40%. In fact, this temperature can be interpreted as the pre-melting temperature. At 1283 K, a structural transition occurs associated with a change in the quasi-equilibrium shape: polyhedron → sphere. There is actual alignment of the fcc and hcp local phases of 19 and 20%, respectively, i.e. the degree, if it decreases, is not significant.

T, K	Chemical segregation	Structural segregation*	
		PTM	AJA
450			
605			

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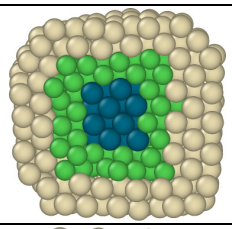
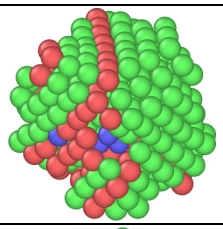
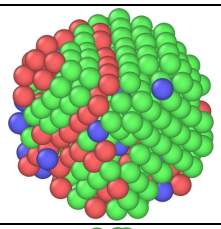
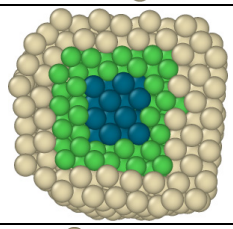
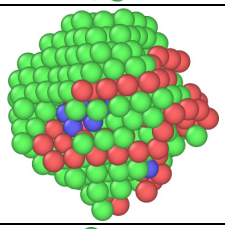
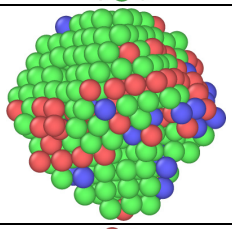
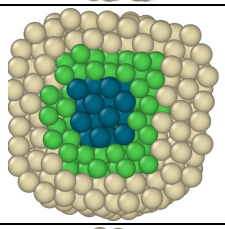
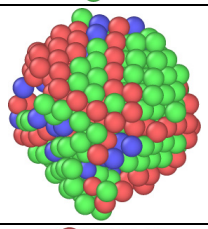
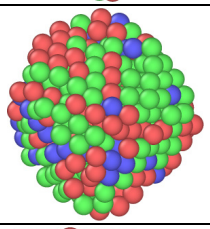
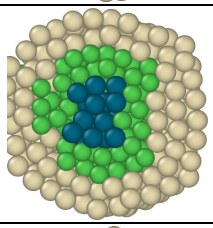
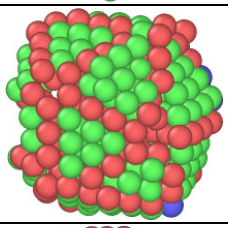
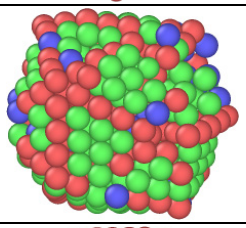
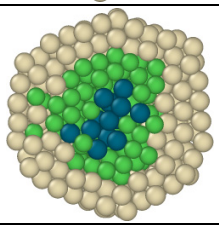
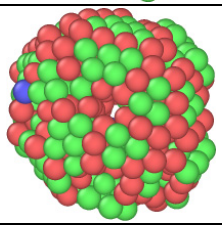
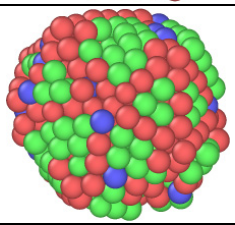
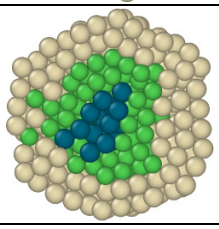
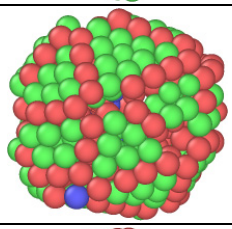
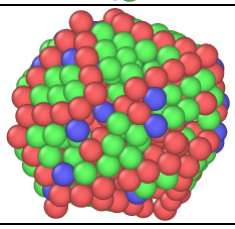
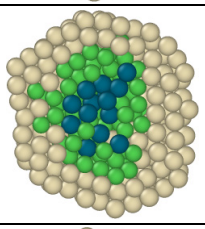
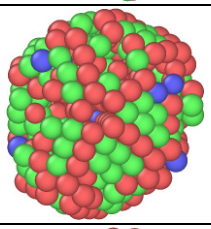
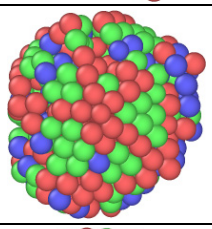
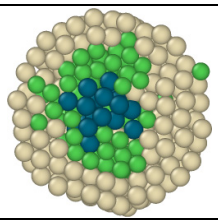
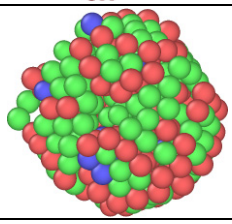
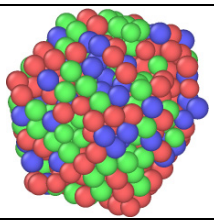
655			
776			
843			
850			
935			
1080			
1200			
1283			

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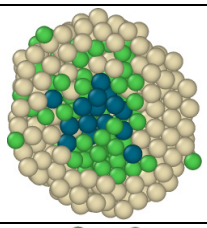
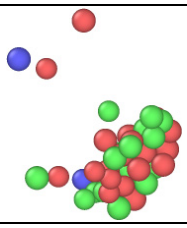
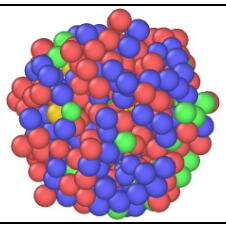
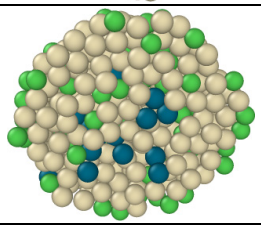
1301			
1360		-	

Fig. 3. Evolution of structural and chemical segregation under thermally induced stress in a ternary $Pd_4@Ni_2@Pt_2$ nanocube. Cross-sections of instantaneous configurations are shown for definite temperatures. Color coding for atom types corresponds to fig. 1. The local environment is designated as follows: green atoms represent the fcc local environment, red atoms represent the hcp local environment, blue atoms represent the bcc local environment, and yellow atoms represent nuclei with icosahedral symmetry. Nuclei unrecognized by the Ovito program [13] have been removed (* – the configuration has been rotated for a better visualization).

At 1301 K, a complete destruction of the local structure (less than 5%) identified by the PTM modifier occurs, while the AJA modifier identifies the local hcp and bcc structures as dominant (more than 31%), which once again proves its inapplicability in the high-temperature region near the phase transition corresponding to melting. The chemical segregation process is complete for nickel atoms at 1360 K. Palladium atoms are identified on the surface.

3. Conclusion

Thus, we have conducted a fairly detailed study of the structural evolution of $Pd_4@Ni_2@Pt_2$ nanocubes during their heating from 300 to 2000 K. In particular, we were interested the patterns of the chemical and structural segregation. Under the chemical segregation, we mean the spatial separation of components, and under the structural segregation the division of the nanoparticle into local regions corresponding to a specific crystal structure. Particular attention was paid to the analysis of the temperature dependence of the potential contribution to the specific internal energy and its relationship with structural transformations, which are usually accompanied by jumps in this dependence. However, a consistent solution to the problem at hand was not possible without direct observation of the evolution of the nanoparticle morphology at the atomic level. Such observation was carried out using the Ovito program [13]. To identify the local environment, two alternative approaches were used for the first time: the polyhedral template method and the Ackland-Jones method. The identification results using both methods are generally in good agreement with

each other, but there are also interesting differences discussed in the previous section.

Due to the pronounced nonequilibrium nature of the initial structure, the thermally induced transformations occurring in it turned out to be quite complex for identification. Nevertheless, we identified several types of transitions: fcc/hcp structural transitions, order/disorder transitions associated with competition between identified and unidentified crystalline phases, sphere-polyhedron transitions, and a melting phase transition. This transition can be considered a first-order phase transition of a complex type, with an atypical behavior of the temperature dependence of the specific potential energy. Although the sharp jump in $u(T)$ occurs in a fairly narrow temperature range, analysis of the structure using the Ovito program [13] showed that melting begins long before this jump.

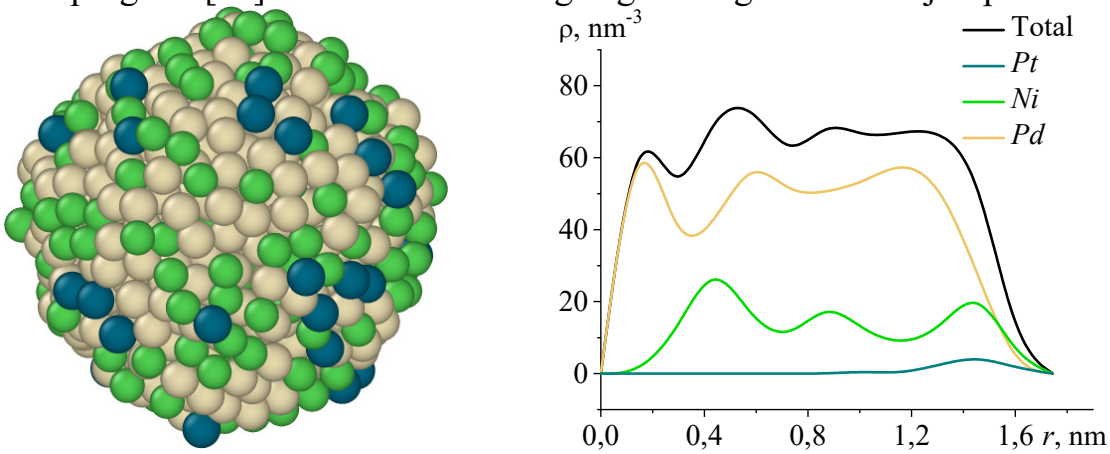


Fig. 4. a – final configuration (volumetric view), b – radial density distributions of components in a ternary $Pd-Ni-Pt$ nanoparticle at a temperature of 2000 K.

From an applied point of view, it is of interest that Pt atoms remain on the surface of $Pd_4@Ni_2@Pt_2$ nanoparticles at all stages of their evolution. Apparently, this is due to the fact that the proportion of Pt atoms in such nanoparticles is the highest (70%). However, after melting, all three components are present in the outer monolayer, including palladium atoms, although their proportion in the nanoparticles under consideration is very small (3,7%). In $Pt_{5000}Pd_{5000}Ni_{5000}$ nanoparticles of larger size and equiatomic composition, platinum atoms were completely absent in the outer monolayers of high-temperature configurations [10]. The described patterns of chemical segregation are confirmed by the data presented in fig. 4. Thus, we have shown that by controlling the final heating temperature of the nanocubes, it is possible to vary the morphology, catalytic properties, and segregation behavior of these nanoparticles. Obviously, the edges and vertices of polyhedra (even those of far from ideal geometric shape) can also have a positive effect on the catalytic activity of both the original nanoparticles and nanocubes that have been significantly transformed during their heating.

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