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Evolutionary prediction and experimental identification of stable phases in Pd–Ni/γ-Al_2O_3 bimetallic catalysts

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Abstract. This work presents a combined theoretical and experimental study of the structural features of Pd–Ni bimetallic nanoclusters. A comprehensive exploration of the configurational space of Pd–Ni nanoclusters (13–56 atoms) across a wide range of compositions (Pd:Ni = 1:1 – 50:1) was performed using the evolutionary algorithm USPEX in conjunction with density functional theory (DFT) calculations. Our approach revealed thermodynamically stable and metastable intermetallic phases with a low-symmetry triclinic structure (space group P1), characterized by complex atomic ordering and a propensity for segregation. The predicted structures were used for a detailed interpretation of experimental X-ray diffraction (XRD) data, enabling the identification of the phase composition of synthesized Pd–Ni/γ-Al_2O_3 samples. We demonstrate that the phase equilibrium in the system non-linearly depends on the overall component ratio, encompassing both single-phase states (e.g., Ni-Pd13 at Pd:Ni = 1:1 and Ni-Pd33 at 10:1) and regions of phase coexistence (e.g., Ni-Pd50 and Ni-Pd33 at 5:1). These findings elucidate the atomistic origins of the synergistic interaction between Pd and Ni and provide a foundation for the rational digital design of highly efficient and selective bimetallic catalysts.

Keywords: bimetallic nanoclusters, Pd–Ni, USPEX, low-symmetry phases, intermetallic phases

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Научная статья
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Эволюционное прогнозирование и экспериментальная идентификация стабильных фаз в биметаллических катализаторах Pd–Ni/γ-Al_2O_3

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Аннотация. Проведено комплексное теоретико-экспериментальное исследование структурных особенностей биметаллических нанокластеров Pd–Ni. С использованием эволюционного алгоритма USPEX в сочетании с методами теории функционала плотности (DFT) выполнено всестороннее изучение конфигурационного пространства нанокластеров Pd–Ni (13–56 атомов) в широком диапазоне составов (Pd:Ni = 1:1 – 50:1). Выявлены термодинамически стабильные и метастабильные интерметаллические фазы с низкосимметричной триклинной структурой (пр. гр. P1), которые характеризуются сложным атомным упорядочением и склонностью к сегрегации. На основе предсказанных структур выполнена детальная интерпретация экспериментальных данных рентгеновской дифракции, что позволило идентифицировать фазовый состав синтезированных образцов Pd–Ni/γ-Al_2O_3. Показано, что фазовое равновесие в системе нелинейно зависит от общего соотношения компонентов и включает как монофазные состояния (например, Ni–Pd13 при Pd:Ni = 1:1 или Ni–Pd33 при 10:1), так и области сосуществования нескольких фаз (например, Ni–Pd50 и Ni–Pd33 при 5:1). Полученные результаты раскрывают атомистические основы синергетического взаимодействия Pd и Ni и закладывают основу для рационального цифрового проектирования высокоэффективных и селективных биметаллических катализаторов.

Ключевые слова: биметаллические нанокластеры, Pd–Ni, USPEX, низкосимметричные фазы, интерметаллические фазы

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Introduction

Bimetallic catalysts are widely employed in heterogeneous catalysis due to their ability to fine-tune catalytic properties, including activity, selectivity, and stability, which are often unattainable in monometallic systems. The synergistic interaction between the two metals allows for the modulation of the electronic and geometric structure of active sites, opening up broad possibilities for the rational design of highly efficient catalytic materials. Among them, palladium-nickel (Pd-Ni) nanoalloys attract particular attention due to their unique combination of palladium's high capacity for activating hydrogen molecules and certain organic substrates, and nickel's low cost and electronic-structural flexibility. The interaction between the components leads to the emergence of ligand and strain effects in the crystal lattice, which modulate the geometry and electronic structure of the active centers [1–3]. Owing to this synergy, Pd-Ni catalysts demonstrate high efficiency in a number of technologically important processes, including the selective hydrogenation of nitroarenes and alkynes [4], the hydrogen evolution reaction (HER) and formic acid oxidation reaction (FAOR) [5], as well as the catalytic hydrolysis of chemical hydrides (e.g., $NaBH_4$) for on-demand hydrogen generation [6].

However, the catalytic properties of Pd-Ni systems are extremely sensitive to their nanostructure, specifically, to the atomic distribution, surface composition, propensity for segregation, and morphology of the nanoclusters. Even with a fixed component ratio and total number of atoms, the configurational space includes thousands of possible isomers, ranging from structures with a Pd shell and Ni core to homogeneous alloys or phase-separated aggregates [7]. Minor variations in these characteristics can drastically alter the adsorption energies of key reaction intermediates (e.g., H, CO, OH), thereby modifying the catalytic pathways or completely deactivating the active sites. Traditional experimental synthesis typically yields polydisperse mixtures with an undefined atomic distribution, which hinders the establishment of clear structure-property relationships.

Under these conditions, in silico approaches based on first-principles calculations become indispensable. Evolutionary algorithms, particularly USPEX (Universal Structure Predictor: Evolutionary Xtallography), provide a powerful tool for exploring the vast configurational space of nanoclusters and identifying thermodynamically stable (or metastable) structures without a priori assumptions about their morphology [8]. In recent years, USPEX has been successfully applied to predict low-energy structures of bimetallic clusters, including Pd-Ni systems. For instance, Bozdag et al. demonstrated that a combination of USPEX and Density Functional Theory (DFT) can reveal the dependence of the preferred structure on composition in Pd_nNi_m clusters ($n + m \leq 20$), as well as establish a correlation between palladium surface enrichment and the optimal hydrogen binding energy (H) for the Hydrogen Evolution Reaction (HER) [9]. Similarly, Zhu et al. utilized USPEX to identify the thermodynamic driving forces behind the formation of core-shell structures with a Ni core and Pd shell in larger clusters, which helped explain their enhanced selectivity in hydrogenation reactions [10].

However, a systematic investigation of Pd-Ni nanoclusters across a broad range of sizes (from sub-nanometer to ~2 nm) and compositions (Pd:Ni = 1:1 – 50:1), coupled with a detailed analysis of their surface electronic properties and catalytic descriptors, remains an unfinished task. Furthermore, the integration of evolutionary structure prediction with machine learning for screening the catalytic activity of Pd-Ni systems is still in its nascent stage.

In this work, we employ the evolutionary algorithm USPEX in combination with Density Functional Theory (DFT) calculations to comprehensively map the structural landscape of Pd-Ni nanoclusters containing 13 to 56 atoms. We identify the global and local energy minima for a series of stoichiometries and analyze their thermodynamic stability, propensity for segregation, and geometric motifs. The obtained results provide an atomic-level understanding of the synergy mechanisms in Pd-Ni systems and establish a foundation for the rational design of new generations of bimetallic catalysts based on digital materials science.

Materials and methods

The catalyst support (γ-Al_2O_3) with a particle size fraction of 125-250 μm was selected for the synthesis of the bimetallic Pd-Ni catalysts. Prior to synthesis, the support was degassed in a vacuum oven for 24 hours at 120 °C to remove moisture and adsorbed atmospheric contaminants. The precursors—palladium acetylacetonate ($Pd(C_5H_7O_2)_2$) and nickel acetylacetonate ($Ni(C_5H_7O_2)_2$)—were dissolved in glacial acetic acid and stirred for 18-24 hours. The resulting powders were then evacuated for 24 hours and subjected to a three-stage thermal treatment under different atmospheres: argon (525 °C, heating rate 1 °C/min), oxygen (375 °C, heating rate 1 °C/min), and hydrogen (525 °C, heating rate 1 °C/min). The dwell time at each stage under the respective gas flow was 2 hours.

The phase composition identification and crystallographic parameter refinement of the synthesized nanostructures were performed using X-ray diffraction on a Miniflex 600 diffractometer (Rigaku, Tokyo, Japan) in Bragg-Brentano geometry with Cu Kα radiation ($\lambda = 1.54178$ Å). Measurements were carried out in the 2θ range of 10–90° with a step size of 0.02° and a counting time of 2 seconds per step. The diffraction data processing and full-profile analysis were conducted using the Rietveld method. The quality of the fit to the experimental data was assessed using the reliability factor R_{wp}.

The lattice parameter for the Pd phase was determined by applying a scale correction to the 2θ axis:

$$2\theta_2 = 2\sin^{-1}\frac{\sin 2\theta_1}{\xi},$$

where $2\theta_1$ is the peak position before refinement, $2\theta_2$ is the peak position after refinement, and ξ is the parameter characterizing the degree of compression or stretching of the unit cell relative to the initial values. Thus, after refining the scale parameter ξ, the lattice parameter was calculated.

The lattice parameter for the Pd phase was refined by correcting the 2θ scale using a scale factor:

$$a_{refined} = \xi * a_{initial}.$$

The experimental diffractograms were described using a model incorporating three main contributions:

$$I_{calc}(2\theta) = \sum_{i=0}^{5} a_i \cdot 2\theta^i + S_{SPT} I_{SPT}(2\theta) + S_{CTLST} I_{\Sigma}(2\theta, \mu, \sigma),$$

where the first term is a polynomial background $a_0, \dots, a_5$ (6th degree), $S_{SPT} I_{SPT}(2\theta)$ is the contribution from the diffraction pattern of the support (γ-Al_2O_3), and $S_{CTLST} I_{\Sigma}(2\theta, \mu, \sigma)$ is the contribution from the catalyst nanoparticles.

Optimization of the 11 model parameters (background coefficients, scale factors, particle size distribution parameters μ and σ, lattice scale factor ξ) was performed using the *curve_fit* module from the *SciPy* library in the *Python* programming environment.

The agreement between the calculated and experimental diffraction patterns was assessed using the weighted profile R-factor, R_{wp}, adjusted for the background intensity:

$$R_{wp} = \left[\frac{\sum_i^N w_i (I_{oi} - I_{ci} - I_{bi})^2}{\sum_i^N w_i (I_{oi} - I_{bi})^2}\right]^{1/2} \times 100\%,$$

where I_{oi} is the intensity at the i-th point of the experimental diffractogram of the mixture, I_{ci} is the intensity at the i-th point of the calculated diffractogram, I_{bi} is the background intensity at the i-th point, $w_i = 1/I_{oi}$ is the weight at the i-th point, and N is the size of the analyzed data array.

For the identification of the observed phases and the analysis of their thermodynamic stability, extensive crystallographic databases containing the results of *ab initio* calculations were used: the Open Quantum Materials Database (OQMD) and the Materials Project. These databases provide information on the crystal structure, unit cell parameters, and static lattice energy at 0 K for thousands of inorganic compounds.

An independent prediction of stable crystalline phases with variable composition was additionally performed for the Pd-Fe system using the USPEX code (Universal Structure Predictor: Evolutionary Xtallography). The calculations were carried out on the "Blochin" supercomputer at the International Research Institute of Intelligent Materials, Southern Federal University. The population size was set to 30 structures per generation. The proportions of generational operators were as follows: 50% heredity, 30% random structures, and 20% mutations. A selection rate of 60% of the best structures was used for progression to the next generation. The number of optimization steps (VASP) was set to 6.

All density functional theory (DFT) calculations utilized in the databases and in conjunction with USPEX were performed within the generalized gradient approximation (GGA). Valence electron wavefunctions were expanded in a plane-wave basis set with a high cutoff energy of 330 eV. The convergence criterion for the total energy was set to $\sim 0.5 \times 10^{-6}$ eV/atom, ensuring high accuracy in determining the lattice energies.

The spatial distribution of atoms within the unit cells of the identified phases was visualized using the VESTA crystal structure analysis based on the obtained crystallographic data (unit cell parameters, atomic positions, space group).

Results

The prediction of thermodynamically stable atomic structures of Pd-Ni was performed using the evolutionary algorithm USPEX. The calculations identified a series of energetically favorable phases across a wide composition range, which formed a targeted crystallographic database for the subsequent interpretation of experimental data. The spatial distribution of atoms in the most stable predicted structures is presented in Figure 1.

Analysis of the predicted structures revealed a general trend: all of them are characterized by triclinic symmetry (space group P1) and a complex, often cluster-like, type of atomic ordering. This indicates that in the Pd-Ni system, the formation of low-symmetry intermetallic phases is energetically more favorable than the formation of disordered solid solutions based on an FCC lattice. This structure results in unique local atomic environments, which can act as highly specific active centers.

A comparative analysis of the experimental diffraction patterns with the calculated profiles for the predicted structures allowed for the unambiguous identification of the phase composition in each of the synthesized samples. The results of the quantitative phase analysis are summarized in Table.

For the 1Pd-1Ni sample (Fig. 2), an almost monophasic state corresponding to the predicted Ni-Pd13 structure (97.02%) is observed. The refined lattice parameters demonstrate significant distortion, indicating structural relaxation in the supported state.

In the 3Pd-1Ni sample (Fig. 3), the dominant phase is Ni-Pd38 (56.83%), indicating a high sensitivity of the phase composition to stoichiometry. The significantly lower lattice energy of this phase (-15000.163 eV) compared to Ni-Pd13 confirms its greater thermodynamic stability in this composition range.

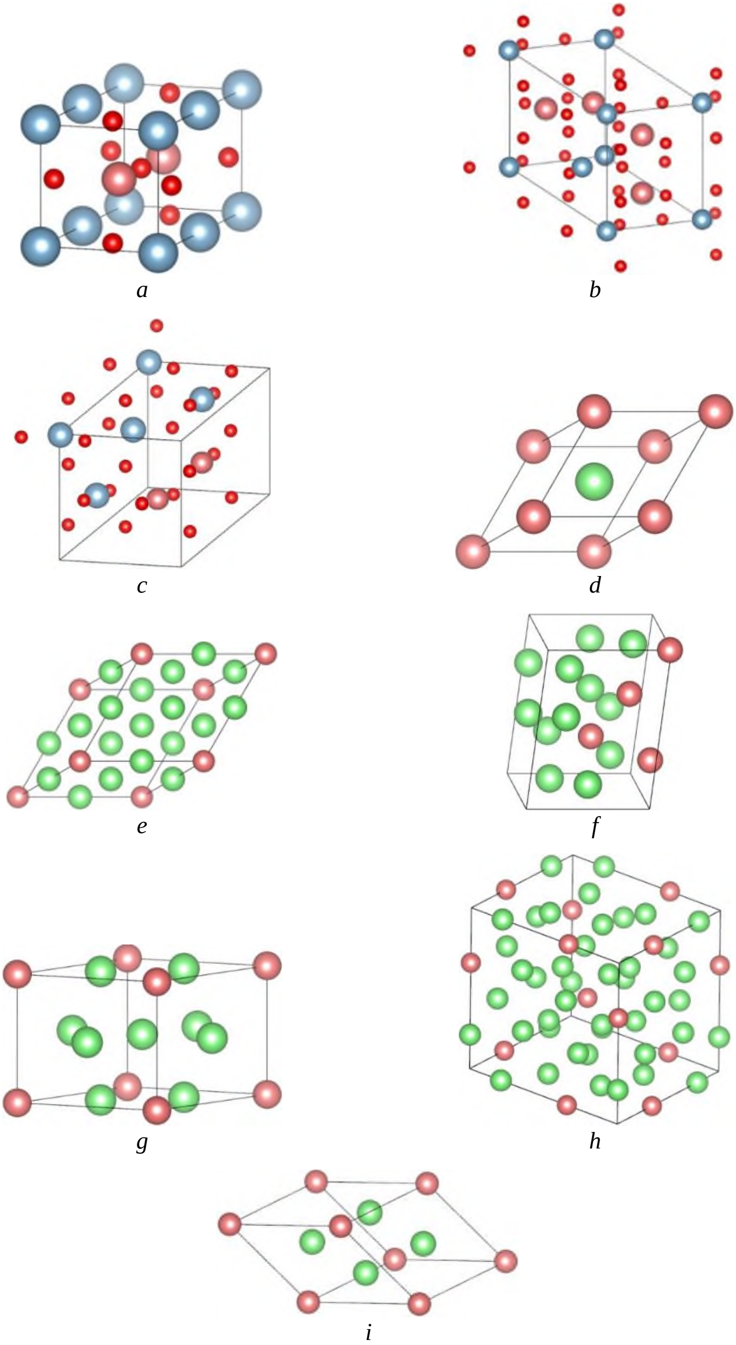

Fig. 1. Atomic structures of the most stable phases in the Pd-Ni system predicted by the USPEX method: *a*) Al2Ni2O5; *b*) Al2Ni2O4; *c*) Al2NiO4; *d*) Ni-Pd13; *e*) Ni-Pd33; *f*) Ni-Pd38; *g*) Ni-Pd50; *h*) Ni-Pd55; *i*) Ni-Pd6

Structural parameters of Pd–Ni samples

Sample	Phase	Lattice Parameters	a, Å	b, Å	c, Å	α, °	β, °	γ, °	E, eV	Space group	Phase content,%	R_{wp}, %
1Pd–1Ni	Ni–Pd13	Initial	3.4791	3.4791	3.4791	60.00	60.00	60.00	–2151.863	P1, Triclinic	97.02	12.48
		Refined	3.5602	3.6602	3.4956	55.97	60.09	65.39	–2151.628			
3Pd–1Ni	Ni–Pd38	Initial	4.7266	6.1461	8.1399	98.88	95.15	97.84	–15000.718	P1, Triclinic	56.83	11.49
		Refined	4.7459	6.2336	8.3263	104.71	93.91	97.97	–15000.163			
5Pd–1Ni	Ni–Pd50	Initial	5.0974	5.0974	4.5237	90.00	90.00	120.00	–5344.687	P1, Triclinic	67.76	10.36
		Refined	5.3809	5.1272	4.6712	86.88	92.41	125.01	–5344.346			
	Ni–Pd33	Initial	5.5295	5.5295	5.5295	60.00	60.00	60.00	–6944.751	P1, Triclinic	30.49	
		Refined	5.5761	5.5761	5.5108	59.19	61.09	63.49	–6944.304			
10Pd–1Ni	Ni–Pd33	Initial	5.5295	5.5295	5.5295	60.00	60.00	60.00	–6944.751	P1, Triclinic	92.515	10.42
		Refined	5.2970	5.6601	5.6810	61.20	61.95	60.76	–6944.400			
	Ni–Pd55	Initial	7.9625	7.9625	7.9625	109.471	109.471	109.471	–22985.381	P1, Triclinic	4.492	
		Refined	8.6819	8.0706	7.9098	105.23	109.08	113.63	–22982.975			
20Pd-1Ni	Ni-Pd50	Initial	5.0974	5.0974	4.5237	90.00	90.00	120.00	–5344.687	P1, Triclinic	95.35	10.22
		Refined	5.1687	5.0521	4.5135	90.28	93.05	120.68	–5344.621			
Ni	Al_2NiO_4	Initial	5.6254	5.6814	5.6814	90.08	119.67	119.67	–6442.218	P1, Triclinic	82.65	12.42
		Refined	5.5291	5.5976	5.4871	90.67	120.21	119.54	–6441.119			
	$AlNi_2O_4$	Initial	5.6883	5.6883	5.6883	120.00	90.00	120.00	–6441.974	P1, Triclinic	7.81	
		Refined	5.7050	5.7051	5.6992	118.52	118.48	61.57	–9026.42			
	$Al_2Ni_2O_5$	Initial	7.5182	3.5278	3.5278	90.00	90.00	90.00	–5004.029	P1, Triclinic	4.40	
		Refined	7.5182	3.5278	3.5223	90.00	90.00	90.00	–5004.02			

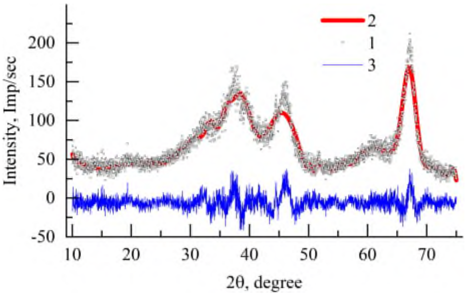

Fig. 2. Diffractogram of the 1Pd-1Ni/Al_2O_3 sample:
1 – experimental; *2* – model; *3* – difference between the curves

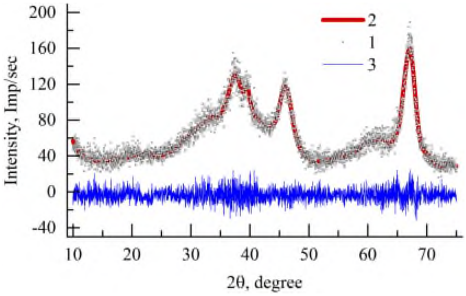

Fig. 3. Diffractogram of the 3Pd-1Ni/Al_2O_3 sample:
1 – experimental; *2* – model; *3* – difference between the curves

The most complex pattern is observed for the 5Pd-1Ni sample (Fig. 4), where the system reaches a two-phase equilibrium between Ni-Pd50 (67.76%) and Ni-Pd33 (30.49%). The presence of two competing phases with comparable fractions indicates the proximity of their formation energies under the given synthesis conditions.

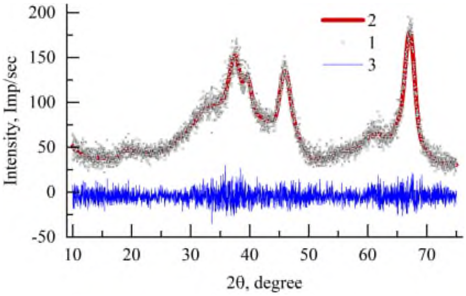

Fig. 4. Diffractogram of the 5Pd-1Ni/Al_2O_3 sample:
1 – experimental; *2* – model; *3* – difference between the curves

In the 10Pd-1Ni sample (Fig. 5), the system again transitions to a state with a single dominant phase—Ni-Pd33 (92.52%). Notably, a minor phase of Ni-Pd55 (4.49%) is present, which exhibits an anomalously low lattice energy (-22982.975 eV). Despite its small fraction, this indicates its exceptional thermodynamic stability.

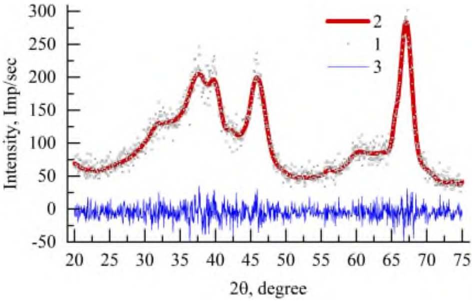

Fig. 5. Diffractogram of the 10Pd-1Ni/Al_2O_3 sample:
1 – experimental; *2* – model; *3* – difference between the curves

With a further increase in palladium content (20Pd-1Ni), the Ni-Pd50 phase (95.35%) becomes dominant (Fig. 6), but with lattice parameters different from those in the 5Pd-1Ni sample, which may indicate polymorphism.

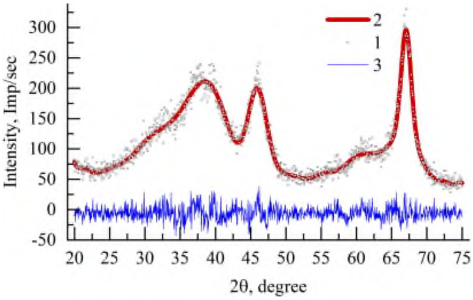

Fig. 6. Diffractogram of the 20Pd-1Ni/Al_2O_3 sample:
1 – experimental; *2* – model; *3* – difference between the curves

It should be separately noted that in the control sample Ni/Al_2O_3 (Fig. 7), nickel aluminate phases (Al_2NiO_4, $AlNi_2O_4$, $Al_2Ni_2O_5$) were identified. This proves a strong chemical interaction between nickel and the support, which must be taken into account when assessing the actual composition of the active bimetallic particles.

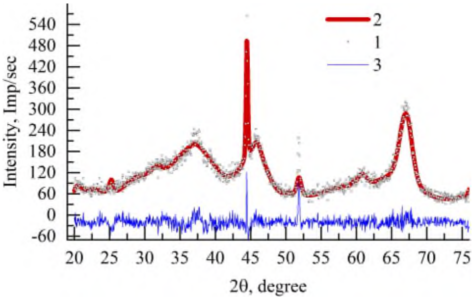

Fig. 7. Diffractogram of the Ni/Al_2O_3 sample:
1 – experimental; *2* – model; *3* – difference between the curves

Conclusions

The combined use of evolutionary prediction (USPEX) and X-ray phase analysis established that an ensemble of discrete intermetallic phases with complex, low-symmetry structures (Ni-Pd13, Ni-Pd33, Ni-Pd38, Ni-Pd50, Ni-Pd55) forms in the Pd-Ni/γ-Al_2O_3 system. Their composition non-linearly depends on the overall component ratio and includes regions where several phases coexist. The calculations confirmed the high thermodynamic stability of the palladium-enriched phases (Ni-Pd33, Ni-Pd55), and their unique atomic ordering suggests the formation of highly specific active sites, opening prospects for the targeted design of selective catalysts.

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