Short communication

On the energetics of vacancy formation and diffusion in mesoporous materials

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Abstract: This paper examines the dependence of the vacancy formation energy and the activation energy of volume diffusion in the «skeleton» of a mesoporous material on the geometric characteristics (volume and shape) of the pores distributed within the material. The geometric features of the pores were defined within a fractal-geometric approach by their effective diameter and fractal dimension. The presented estimates indicate that the effect characteristic of nanoparticles, associated with the significant dependence of the vacancy formation energy and the activation energy of volume diffusion on the particle size and shape, can also occur in mesoporous materials (with a characteristic pore size from 5 to 50 nm), even though the mesoporous objects themselves can have macroscopic dimensions. Using porous gold as an example, it is shown that a decrease in the pore volume and a «complication» of their morphology lead to a noticeable reduction in the considered energy characteristics. The results were obtained within the framework of the cohesive energy-based model.

Keywords: vacancy formation energy, volume diffusion activation energy, mesoporous materials, fractal dimension, cohesion, size distribution, Hardy-Ramanujan-Rademacher formula.

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К вопросу об энергии образования вакансии и энергии активации диффузии в мезопористых материалах

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Аннотация: В данной работе рассмотрена зависимость энергии образования вакансии и энергии активации объемной диффузии в «скелете» мезопористого материала от геометрических характеристик (объема и формы) распределенных в материале пор. Геометрические особенности пор задавались в рамках фрактально-геометрического подхода величинами их эффективного диаметра и фрактальной размерности. Приведенные оценки свидетельствуют о том, что характерный для наноразмерных частиц эффект, связанный с существенной зависимостью энергий образования вакансии и активации процесса объемной диффузии от размера и формы частицы, может также реализовываться в мезопористых (характерный размер пор от 5 до 50 нм) материалах, при том что сами мезопористые объекты могут иметь макроскопические размеры. На примере пористого золота показано, что уменьшение объема пор и «усложнение» их морфологии приводят к заметному снижению рассматриваемых энергетических характеристик. Результаты получены в рамках когезионной модели.

Ключевые слова: энергия образования вакансии, энергия активации объемной диффузии,

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мезопористые материалы, фрактальная размерность, когезия, распределения по размерам, формула Харди-Рамануджана-Радемахера.

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Structures with small characteristic sizes and functional materials based on them exhibit unique physicochemical properties that have been the subject of intensive scientific research over the past few decades [1, 2]. For metals and inorganic compounds, most of these properties manifest themselves when the characteristic size of the structural elements reach the submicron and nanometer range. For particles of small volume, a significant dependence has been established of the temperatures of the first-order (melting [1-3]) and second-order phase transitions (magnetic transformations [4], transition to the superconducting state [5]), the characteristic Debye temperature, transport properties, the vacancy formation and the diffusion activation energies [6], as well as a number of mechanical properties, on geometric parameters, with the absolute values of these quantities differing significantly from the corresponding values for macroscopic samples. In multicomponent systems, the mutual solubility of components, the liquidus and solidus temperatures, and the equilibrium composition of coexisting phases in heterogeneous regions depend on the particle morphology, and specific effects are also observed (the «initial composition» effect, «external environment» effect, «hysteresis effect», and others) [7-10], which can be explained within the framework of thermodynamic and other approaches [3]. These features are largely due to the increasing fraction of surface low-coordinated atoms, whose characteristics differ from those of bulk atoms, as the size of structures decreases and their morphology becomes more complex. In other classes of systems (e.g., polymers), similar effects appear in different size ranges, including the range accessible to visual observation [11]. The realization of such effects in small particles and composite materials based on them opens up possibilities for the targeted control of functional characteristics, which should be taken into account when developing synthesis methods.

Previously, we noted that high specific surface areas can be achieved not only in nanopowder materials and composites based on them, but also in mesoporous objects with effective pore diameters from 5 to 50 nm [12]. In such materials, the set of physicochemical properties begins to be largely determined by pore morphology. The present work is the final one in a series of studies [12-15] and is devoted to the study of the energy characteristics of vacancy formation and diffusion activation in the «skeleton» of a mesoporous material

using pure mesoporous gold as an example. In our previous papers, we considered the influence of pore morphology on the Curie temperature of mesoporous ferromagnets [12], the normal elastic modulus (Young's modulus) [13], the melting temperature of mesoporous metals [14], and the electron-optical characteristics of semiconductor crystals [15].

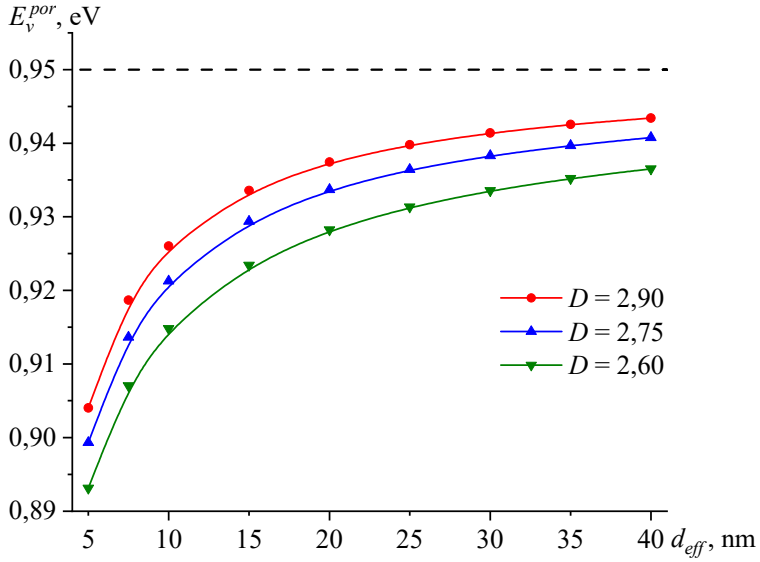

Fig. 1. Estimated dependence of the vacancy formation energy E_v^{por} for mesoporous gold on pore morphology (effective diameter d_{eff} and fractal dimension D).

The basis for the model developed below is the relationship – described, for example, by the authors of [16-18] and a number of other works – between the vacancy formation and bulk diffusion activation energies and the material's cohesive energy (a comparison of the obtained dependences using the example of nanoparticles of a number of metals, including gold, with experimental data, as well as with alternative modeling approaches [19-21], showed satisfactory agreement. Below, gold is used as a model material as well): $E_v^{por}/E_v^{bulk} = E_{coh}^{por}/E_{coh}^{bulk}$ and $E_A^{por}/E_A^{bulk} = E_{coh}^{por}/E_{coh}^{bulk}$. Here, E_v^{por} and E_A^{por} are the vacancy formation energy and diffusion activation energy of the porous material, respectively; E_v^{bulk} and E_A^{bulk} are the vacancy formation and diffusion activation energies of the material in the absence of pores, respectively; E_{coh}^{por} and E_{coh}^{bulk} are the cohesive energies of these materials. Nanostructuring (whether it is the formation of nanoparticle ensembles or mesoporous structures) is accompanied by a significant increase in the fraction of surface-layer atoms with dangling bonds, which leads to a noticeable change in the cohesive energy and related characteristics [5, 6, 12-15]. To estimate the cohesive energy of continuous macroscale structures and mesoporous materials, the relationships proposed by F. Aqra and A. Ayyad [22] can be used:

$$E_{coh}^{bulk} = \frac{1}{2}\beta N\varepsilon_b, \quad E_{coh}^{por} = \frac{1}{2}\beta\varepsilon_b\left(\frac{1}{4}N_s + \left(N - N_s\right)\right). \qquad (1)$$

Here, N is the number of atoms per 1 g of the material, N_s is the number of atoms located on the pore surface, ε_b is the energy of a single bond in the crystal; β is the first coordination number.

The complex and irregular morphology of real porous materials can be described using two parameters: the effective pore diameter d_{eff} numerically equal to the diameter of a sphere whose volume equals the volume of the pore under consideration, and the fractal dimension of the pore D. The latter parameter is used by us analogously to [12-15] and defines the relationship between the pore volume $V = \pi d_{eff}^3/6$ and the pore surface area A: $A = C\left(\pi d_{\text{eff}}^3/6\right)^{2/D}$ (for more details on the use of D as a structural characteristic, see [23-25]). As in, for example, [12-15, 25], without loss of generality we set $C = 4\pi$. One of the main advantages of the proposed approach is that the presented parameters generalize different pore morphologies, having the same values for geometrically dissimilar structures that, however, share the same surface area-to-volume ratio and the same fraction of surface-layer atoms.

Let the volume fraction of pores in the mesoporous material be α. If d_{at} is the atomic diameter, ρ is the density of the material, and ω is the volume packing density of the crystal structure of the material, then for the total number of atoms contained in 1 g of the material we obtain $N = 6\omega \cdot 1\ \text{g}/\left(\pi d_{at}^3 \cdot \rho\right)$ where the factor 1 g is introduced for dimensional consistency. For the number of atoms on the pore surface in 1 g of mesoporous material, we also obtain $N_s = 6\alpha\eta k \cdot 1\ \text{g}/\left(\pi\rho d_{at}^2 d_{eff}\right)$ where η is the volume packing density of the crystal structure of the material under consideration. The value k has the geometric meaning of the ratio of the surface area of a structure with fractal dimension D to the surface area of a sphere of the same volume and is calculated as $k = C(\pi/6)^{2/D-1} d_{eff}^{6/D-3}$. Thus, for the dependence $N_s(N)$ at given α, d_{eff}, and D, we have:

$$N_s(N) = \left(6 \cdot 1\ \text{g}/\pi\rho\right)^{1/3} \cdot \left(\alpha\eta k/\omega^{2/3} d_{eff}\right) \cdot N^{2/3}. \qquad (2)$$

Directly substituting (2) into (1) after a series of algebraic transformations yields

$$E_{coh}^{por} = \frac{1}{2}\beta N\varepsilon_b\left(1 - \frac{3}{4}C \cdot (1\ \text{g}/\rho)^{1/3} \cdot \left(\alpha\eta/\omega^{2/3}\right) \cdot (\pi/6)^{2/D-4/3} \cdot d_{eff}^{6/D-4} \cdot N^{-\frac{1}{3}}\right),$$

$$E_v^{por} = E_v^{bulk}\left(1 - \frac{3}{4}C \cdot (1\ \text{g}/\rho)^{1/3} \cdot \left(\alpha\eta/\omega^{2/3}\right) \cdot (\pi/6)^{2/D-4/3} \cdot d_{eff}^{6/D-4} \cdot N^{-\frac{1}{3}}\right), \qquad (3)$$

$$E_A^{por} = E_A^{bulk}\left(1 - \frac{3}{4}C \cdot (1\ \text{g}/\rho)^{1/3} \cdot \left(\alpha\eta/\omega^{2/3}\right) \cdot (\pi/6)^{2/D-4/3} \cdot d_{eff}^{6/D-4} \cdot N^{-\frac{1}{3}}\right).$$

The calculations below (see Fig. 1 for the vacancy formation energy and Fig. 2 for the bulk diffusion activation energy) are performed for mesoporous

gold having an *fcc* structure over the entire temperature range up to the melting temperature. The structural characteristics for the *fcc* lattice, according to [18], are $\omega = 0,74$, $\eta = 0,91$. For Au, $d_{at} = 288$ pm, $E_v^{bulk} \approx 0,95$ eV [16], $E_A^{bulk} \approx 108$ kJ/mol [17]. The density of gold is estimated as $\rho \approx 19,32$ g/cm^3. Although modern methods for producing porous structures make it possible to achieve extremely high specific surface areas (from 500 m^2/g up to 1000 m^2/g and even several thousand m^2/g, see [12-15] and references therein), in the present calculations we restrict ourselves to not too high specific surface areas, not exceeding 200-300 m^2/g, which corresponds to a value of $\alpha = 0,85$. From Figs. 1-2 it can be seen that the magnitudes $\left|\partial E_v^{por} / \partial d_{eff}\right|$ and $\left|\partial E_A^{por} / \partial d_{eff}\right|$ increase as d_{eff} decreases. In mesoporous materials, the key reason for the reduction in vacancy formation energy and bulk diffusion activation energy is the «loosening» of the crystal structure caused by the proximity of the free surface. Surface atoms on the pore walls experience asymmetric interatomic interactions (lack of neighbors on the inner side), which leads to the weakening of bonds in the near-surface layers and an increase in average interatomic distances – the structure becomes less rigid, and less work is required to create a vacancy. Furthermore, the surface acts as an effective sink and source of vacancies, further lowering the energy barrier for their formation. In addition, for more accurate quantitative modeling, it is possible to account for the high Laplace pressure (which may complicate diffusion but does not eliminate the dominance of surface loosening in mesoporous materials), as well as the increased fraction of atoms with a reduced coordination number, which together reduce the activation energy for vacancy migration, accelerating bulk diffusion compared to dense materials.

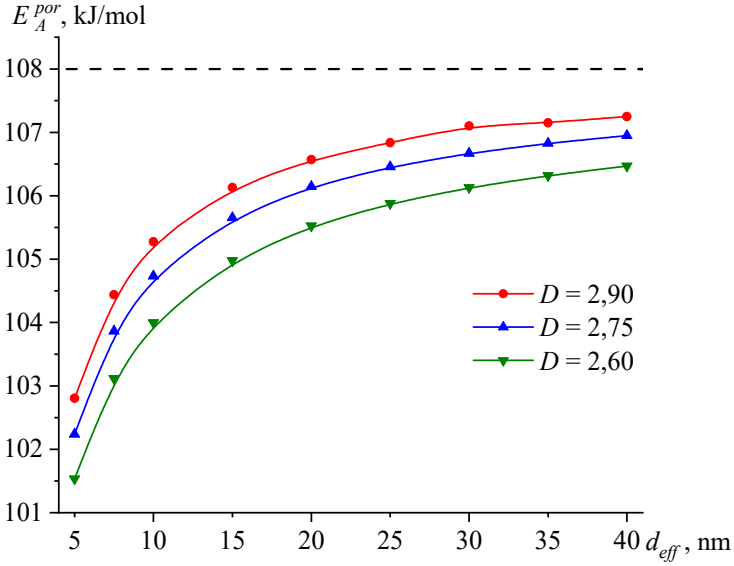

Fig. 2. Estimated dependence of the bulk diffusion activation energy E_A^{por} for mesoporous gold on pore morphology (effective diameter d_{eff} and fractal dimension D).

The results obtained above can be generalized by transitioning from «monomorphological» mesoporous materials to «polymorphological» ones, characterized by pore distribution functions with respect to morphological characteristics. The set of numerous experimentally obtained pore distributions of this kind (see, for example, in [26]) suggests that mathematically they can be described by adapting approaches originally proposed in [25, 27, 28]. In that case, the mean values of the pore fractal dimension $\langle D \rangle$, the effective diameter $\langle d_{eff} \rangle$, and the mean «stoichiometric number» [27, 28] of the pore $\langle \phi_p \rangle$ (the number of atoms required to «fill» the pore until a regular continuous structure is formed, $\phi_{por} = \omega \left(d_{eff} / d_{at} \right)^3$) are calculated as [13, 25]:

$$\langle D \rangle = \frac{\sum_i D_i \int f_D \left(D_i, \phi_{por}, N \right) d\phi_{por}}{\Omega(N)}, \quad \langle \phi_p \rangle = \frac{\sum_i \int \phi_{por} f_D \left(D_i, \phi_{por}, N \right) d\phi_{por}}{\Omega(N)}, \tag{4}$$
$$\langle d_{eff} \rangle = \Omega(N)^{-1} d_{at} \sum_i \int f_D \left(D_i, \phi_{por} \right) d\phi_{por}, \quad \Omega(N) = \sum_i \int f_D \left(D_i, \phi_{por}, N \right) d\phi_{por},$$

where $f_D \left(\phi_{por}, D, N \right)$ are pore size distribution functions for pores with fractal dimension D, obtained using partition theory and an asymptotic estimate for the Hardy-Ramanujan-Rademacher formula [25, 27-28]:

$$f_D \left(\phi_{por}, D, N \right) \sim \exp\left(-\frac{U\left(\phi_{por}, D \right) + RT \ln f_{por}}{RT} \right), f_{por} = \frac{N}{N - \phi_{por}} \exp\left\{ \pi \left(\sqrt{\frac{2}{3}} \left(N - \phi_{por} \right) - \sqrt{\frac{2}{3} N} \right) \right\}. \tag{5}$$

Here, $U\left(\phi_{por}, D \right)$ is the energy characteristic of defect (pore) formation with given stoichiometric number and fractal dimension (for more details, see [27, 28]). The integration limits in expressions (4) correspond to the range of stoichiometric numbers under consideration, while the summation is performed over a sample of distributions with $D_i \in (2,3)$ and an arbitrarily chosen step.

The obtained quantitative estimates demonstrate the possibility of purposeful control of diffusion properties and defect formation in functional materials through controlled «tuning» of their porous structure. Although calculations are limited to moderate porosity, the general approach is universal and can be easily scaled to other metals and types of nanostructures if appropriate input data are available. The material is particularly interesting for the physical chemistry of nanostructured catalysts and sensors, where diffusive mobility of atoms in the skeleton often determines device performance.

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