USING QUANTUM-MECHANICAL SOLUTIONS TO CALCULATE THE DIFFUSION COEFFICIENTS OF METAL VAPORS IN GASES

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The diffusion of metals in inert gases is calculated on the basis of quantum-mechanical calculations of atomic interactions and the temperature dependence is refined with generalization of the experimental data.

There have now appeared numerous works with quantum-mechanical calculations of the interaction energy of alkali-metal atoms with inert-gas atoms (for ground and excited states), on the basis of the variational solution of the Schrödinger equation in the Born—Oppenheimer approximation of "frozen" nuclei, including both nonempirical calculations that do not employ any experimental parameters [1-4] and semiempirical calculations [5-9]. In the Born—Oppenheimer approximation, the quasimolecule energy E(r) is determined as the sum of the energy of electron motion in the field of the nucleus and the other electrons and the energy of nuclear repulsion. The potential energy of atomic interactions, which may be used in calculations of the transfer coefficients, is determined by the expression

$$\varphi(r) = E(r) - E(\infty),$$

where $E(\infty)$ is the energy of atoms removed to infinity.

Nonempirical calculations are performed by the Hartree—Fock self-consistent-field method. The molecular orbitals are determined by the linear combination of atomic orbitals with basis functions of Slater or Gaussian types (the final results are practically the same for both types of basis function). The computational scheme is based on the use of the Rutaan system of equations, taking into account that the external electron shell of the alkali metal is open (includes one valence electron). In [2], for the pairs of atoms H—He and Li—He, account is also taken of the configurational interaction (leading to large distances between the nuclei for dispersional interaction); however, no calculations are performed for short distances. The calculations of [1] for the pairs of atoms Li—He and Na—He were performed without taking account of configurational interaction, i.e., only the Coulomb interaction of electrons (and nuclei) and the electron exchange interaction were taken into account. The exchange interaction (in this case, repulsive) is a consequence of the Pauli principle of antisymmetry of the electron wave function. It predominates at moderate distances between the atoms (nuclei), corresponding to values of around 10^{-3}-10^{-2} at. units for $\varphi(r)$ (approximately 300-3000°K in temperature units), in contrast to the case of large distances, when dispersional repulsion plays the basic role.

Complete calculation for the atomic pair Na—Ar was performed in [3], both for large and for moderate and small distances between nuclei, taking account of Coulomb, exchange, and configurational interactions (Fig. 1). The contribution of the latter is quite large here, even at small and moderate distances. Conversely, the contribution of configurational interaction for the same distances in the interaction of Li or Na atoms with He atoms is small, since the polarizability of helium is almost an order of magnitude less than that of argon.

Approximate calculations taking account of the interaction of outer-shell electrons and the atomic core separately were performed in [4] for the atomic pairs Na—Ar and Na—Xe (taking account of the configurational interaction). For the atomic pair Na—Ar, $\varphi(r)$ values obtained in [4] are larger by a factor of approximately 1.3 than those in [3].

In semiempirical quantum-mechanical calculations of the atomic interaction performed by the variational methods, particular simplifications are introduced in the Hamiltonian of the

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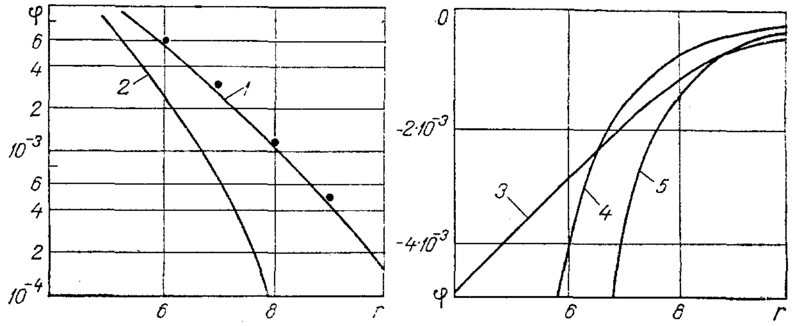

Fig. 1. Potential energy of the interaction of sodium and argon atoms: 1) φ (r) according to the calculations of [3], without taking account of the configurational interaction; 2) the same taking account of the configurational interaction; 3) attractive energy (the difference in the theoretical energies [3] taking account and not taking account of the configurational attraction); 4) dispersional attractive energy $C_6^{Na-Ar}r^{-6}$ ($C_6^{Na-Ar} = 190$ [18]); the same, $C_6^{Na-Ar}r^{-6} + C_8^{Na-Ar}r^{-8}$ ($C_8^{Na-Ar} = 1.27\cdot10^4$ [18]; the points correspond to calculation of φ_{exch} when ρ = 3.1, L = -1.6. Here and in the other figures, all the quantities are expressed in atomic units (at. units).

Schrödinger equation. In [5], the Hamiltonian was written as the sum of the Hamiltonian of the valence electron of the unperturbed alkali-metal atom and the potential energy of the interaction of this electron and the atomic core of the metal with the inert-gas atom. In the expression for this energy, account was taken of the electrostatic interaction of the electron with the inert-gas atom (which is transformed to dispersional attraction at large distances) and the interaction of the electron shells of the given core and atom. The latter was taken into account using a pseudopotential of Gombash type, based on the Thomas–Fermi model of the electron shells and satisfying the Pauli principle. A free parameter selected from the coincidence of the theoretical depth of the potential well (for the ground state) and the experimental value from the data of [10] on scattering of a metallic atomic beam in an inert gas was introduced in the calculation. Improvement of this method in [6] by increasing the number of states taken into account in the atomic basis led to improvement in the results.

There are now a number of semiempirical calculations for the atoms Li–He, Li–Ne, Na–He, and Na–Ne based on using a model potential which takes account of the experimental data on electron scattering at inert-gas atoms and alkali-metal ions in the Hamiltonian [7-9]. The electrostatic interaction is also taken into account.

It is of interest to calculate the diffusion coefficients of alkali-metal vapors (practically monoatomic vapors) in inert gases on the basis of the given quantum-mechanical calculations (nonempirical and semiempirical) and to compare the results with experimental data encompassed by the generalization formulas [1]. Such calculations are performed using a formula based on Enskog–Chapman kinetic theory [12] (in the first approximation of the solution of the Boltzmann equations and the first approximation of calculations in expansions with respect to the Sonine polynomial)

$$PD_{12} = 0.0266\sqrt{T^3(M_1+M_2)/2M_1M_2}/Q_{12}^{(1,1)}, \tag{1}$$

where PD_{12} is expressed in N/sec (D_{12} in m²/sec), and $Q_{12}^{(1,1)}$ in Å².

The theoretical potential-energy curve of the interaction of metal and gas atoms in the ground state for a particular case is approximated by the dependence

$$\varphi(r) = B\exp(-r/\rho), \tag{2}$$

where B and ρ are constants. The use of Eq. (2) taking no account of the potential well in the dependence φ(r) is permissible since the depth of the potential wells is small in comparision with the temperature level in the calculations. For the given potential function, according to [13]

$$Q_{12}^{(1,1)} = 4\alpha^2\rho^2 I(1,\ 1),$$

where I(1, 1) is the collision integral, tabulated in [13] as a function of α = ln(B/kT).

TABLE 1. Values of PD_{12} and n Calculated from the Theoretical Potential for Mixtures of Alkali-Metal Vapors with Inert Gases (d, ratio of theoretical value of PD_{12} and the result of generalization)

Mixture	T_{ref}, K	PD_{12}, N • sec^{-1}	d	n	n_{gen}
Na — Ar [3]	863	11,4	0,80	1,90	1,67
Na — Ar [3]	863	14,8	1,04	1,81	1,67
Na — Ar [4]	863	13,5	0,95	1,85	1,67
Na — Ar [6]	863	12,9	0,90	1,76	1,67
Na — He [1]	863	33,3	0,93	1,96	1,67
Na — He [6]	863	32,4	0,90	1,78	1,67
Na — Ne [7]	863	17,9	0,92	1,89	1,67
Na — Xe [4]	863	9,9	0,88	1,75	1,67
Li — He [1]	1210	88,3	1,13	1,99	1,67
Li — He [6]	1210	84,2	1,07	1,92	1,67
Li — Ne [7]	1210	49,1	0,93	1,90	1,67
Li — Ar [6]	1210	39,8	0,95	1,86	1,67
Li — Kr [6]	1210	37,4	0,96	1,87	1,67
Li — Xe [6]	1210	36,1	0,99	1,84	1,67
Cs — He [6]	707	20,8	1,12	1,73	1,65
Cs — Ar [6]	707	5,5	0,90	1,70	1,65
Cs — Kr [6]	707	4,1	0,87	1,69	1,65
Cs — Xe [6]	707	3,3	0,81	1,67	1,65

Some results of the calculations are shown in Table 1. The values of PD_{12} for mixtures of a particular metal with gases correspond to the reference temperature $T_{ref} = 0.75T_b$, where T_b is the boiling point of the metal at atmospheric pressure (K). The quantity T_{ref} corresponds approximately to the mean temperature of the experiments to determine the diffusion coefficient which provided the reference values in the generalization [11]. These experiments are performed in the temperature range $0.6-0.9T_b$, approximately. Table 1 also gives the values of PD_{12} found for the given generalization, i.e., calculated from Eq. (1) with $Q_{12}^{(1,1)}$ determined from the formula of [11] as a function of the ionization energy of the metal I_1 and the gas I_2 and the polarizability of the gas α_2.

It is evident from Table 1 that, for Na–Ar mixtures, the theoretical value of PD_{12} (row 1) calculated using the potential curve of [3] taking no account of the configurational interaction (Fig. 1, curve 1) is markedly lower than that found using the generalization. However, if the potential curve of [3] that takes account of the configurational interaction is used (Fig. 1, curve 2), the agreement between the values of PD_{12} (second row) is better. Approximately the same level of agreement is found for the generalization and the value of PD_{12} for the given mixture (and with larger deviations for the mixture Na–Xe) found using the potential energy value calculated in [4], taking account of configurational interaction. The values of PD_{12} calculated for Li–He, Na–He using the potential curves of [1] do not differ very much from the generalization, although in these calculations, as noted, no account was taken of the configurational interaction. Satisfactory agreement with the generalization is also found for the values of PD_{12} for Li–He, Li–Ne, Na–He, Na–Ne calculated using the values of the potential-energy of the interaction found in semiempirical calculations [7]. The potential curve of [8] for Na–He is practically the same as that of [1]. Hence the theoretical values of PD_{12} will also be the same. The data of [9] for Na–He cannot be used in diffusion calculations, since in [9] no values of the interaction energies were given for moderate internuclear distances. (The electrostatic interaction corresponding essentially to the configurational interaction is taken into account in all semiempirical calculations, as is clear from the foregoing.) Using the potential energy of atomic interaction obtained by semiempirical calculation in [6] to calculate the diffusion coefficients also leads to values of PD_{12} that agree with the generalization in a number of cases (Table 1). However, the discrepancy may be more considerable (20% or more, for example, for mixtures of K vapor with gases), especially for mixtures with heavy inert gases. For mixtures with neon, the discrepancy is very large (up to 38%). It may be assumed that this is associated with inaccuracy of the calculation of [6] for the given case. As already noted, calculations using the interaction energy calculated by another semiempirical method [7] lead to satisfactory values of PD_{12} for mixtures with neon.

Overall, the agreement between the values of PD_{12} at the reference temperature found using the results of quantum-mechanical calculations and from the generalization of [11] is completely satisfactory. Table 1 also gives values of the exponent n in the temperature de-

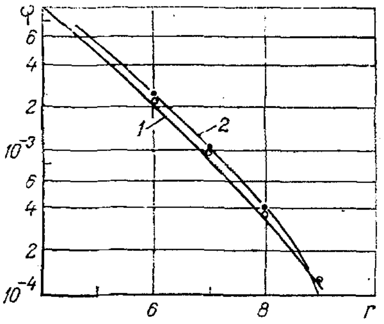

Fig. 2. Potential energy of the interaction of lithium and helium atoms and of sodium and helium atoms: 1) $\varphi(r)$ from the calculations of [1] for Li—He; 2) $\varphi(r)$ from the calculations of [1] for Na—He; the points correspond to calculation of φ_{exch} at $\rho = 0$, $L = 1.2$.

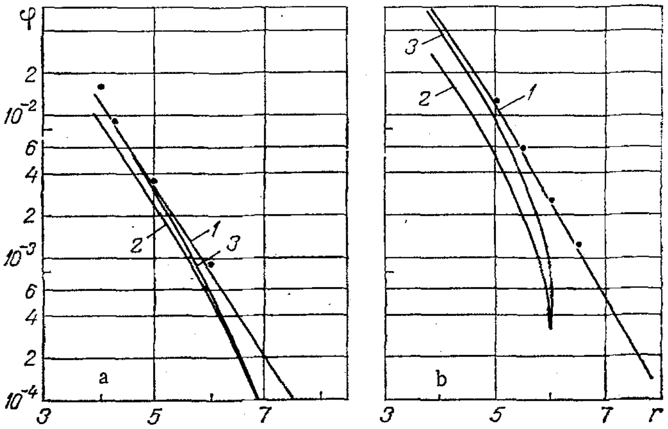

Fig. 3. Potential energy of Hg—He (a) and He—Ar (b) interaction: a) calculation of $\varphi_{exch}(r)$ with $\rho = 0$, $L = 1.2$ (1); $\varphi(r) = \varphi_{exch}(r) - C_6^{Hg-He} r^{-6}$ (2); $\varphi(r) = \varphi_{exch}(r) - \varphi_{at}^{Hg-He}(r)$ with φ_{at}^{Hg-He} defined in Eq. (9) (3); b) calculation of $\varphi_{exch}(r)$ with $\rho = 3.1$, $L = -1.6$ (1); $\varphi(r) = \varphi_{exch}(r) - C_6^{Hg-Ar} r^{-6}$ (3); $\varphi(r) = \varphi_{exch}(r) - \varphi_{at}^{Hg-Ar}(r)$ with $\varphi_{at}^{Hg-Ar}(r)$ defined in Eq. (9); the points correspond to the repulsive energy from the data of [23] on the scattering of a Hg atomic beam.

pendence $PD_{12} \sim T^n$ found from the given theoretical calculations in the temperature range 300-2000°K (n varies weakly with temperature variation — within limits of one or two hundredths), as well as values of the temperature exponent n^{gen} derived from the generalization formula [11]. It is evident that the theoretical values of n are markedly higher than n^{gen}. This is because, as noted earlier, the reference experiments for the generalization were performed in a relatively narrow temperature range, and the value of the temperature exponent cannot be sufficiently accurately determined (especially because of the large spread in experimental values of PD_{12}, amounting to ±10-15%). The theoretical values of n may be regarded as reliable for a considerably broader temperature range; in using these values of n, the deviation of PD_{12} within the experimental limits of temperature variation is considerably less than the experimental error. Thus, for mixtures of alkali-metal vapors with inert gases, it is reasonable to introduce the following correction in the temperature exponent n^{gen}:

$$n = n^{gen} + \Delta, \tag{3}$$

where $\Delta \approx 0.15$-0.2. The results of the generalization may be written in the following form here

$$PD_{12} = C(T/T_{ref})^n. \tag{4}$$

The coefficient C is defined as the value of PD_{12} according to the formula of [11] at the temperature T_{ref} (the value of n^{gen} is retained in calculations of C).

In addition to methods of calculating the atomic interaction on the basis of solving the complete Schrodinger equation, an asymptotic method has been developed, using the appropriately simplified Schrödinger equation for large interatomic distances [14-17]. For the model of a zero-radius potential, the exchange repulsive energy between alkali-metal atoms (with a low ionization potential) and a helium atom is expressed by the asymptotic formula (atomic units are used)

$$\varphi_{\text{exch}}(r) = 2\pi L\Phi^2(r)/(1-\beta' L), \tag{5}$$

where $\beta' = (\beta^2 - 2/r)^{1/2}$; L is the electron scattering length at the helium atom. As $\beta' \to 0$, the well-known Fermi formula is obtained from Eq. (5).

For a more general model in which the finite radius of the spherical integration surface surrounding the perturbing atom with a high potential energy is introduced, the following expression may be written

$$\varphi_{\text{exch}}(r) = 2\pi(L+\rho)\Phi^2(r)(\beta'\rho+1)\frac{\exp(\beta'\rho)}{1-\beta' L}. \tag{6}$$

Equation (5) corresponds to the case when $\rho \to 0$.

The asymptotic wave function of the valence s electron of the metal is determined by the expression [14]

$$\Phi(r) = Ar^{\frac{1}{\beta}-1}\exp(-\beta r)/\sqrt{4\pi}. \tag{7}$$

The value of the coefficient ensuring matching with the Hartree–Fock solution at small r was given for various atoms in [14, 18] (with an accuracy of ±10-20%).

Various values for the electron scattering length at a helium atom are given in the literature: from 1.14 at. units [19] to 1.44 at. units [15]. According to the data of [20], L = 1.28 at. units for helium. Below, a mean value L = 1.2 at. units is used.

Calculating φ_{exch} from Eqs. (5) and (7) for Li–He (for lithium, $\beta = 0.63$ at. units, $A = 0.82$ at. units, $\beta' = 0$ when $r = 5.04$ at. units) leads to satisfactory agreement with the results of nonempirical calculations [1] (Fig. 2) at distances larger than 6-8 at. units, i.e., energies less than 10^{-3}-10^{-4} at. units. The same agreement is obtained in analogous calculations for Na–He. The use of Eqs. (5) and (7) to determine the exchange-repulsion energy of atoms of two-electron metals with helium atoms — for example, mercury, cadmium, zinc atoms — is of particular interest. For such calculations, an additional factor ω must be introduced in Eq. (5), taking account of the difference in spin states of the atoms and the atom and the atomic core (with removal of a single electron) from the corresponding spin states of the alkali-metal atoms and its atomic core. The corresponding calculations by the genealogical scheme of Racah [14, 21] using the formulas for Wigner 9j symbols [22], the Clebsch–Gordan coefficients, and the genealogical coefficients give $\omega = 2$ for the interaction of two-electron metals (with valence s electrons) with helium or other inert gases.

The results of calculating φ_{exch} from Eqs. (5) and (7) with the factor $\omega = 2$ for Hg–He (for mercury $\beta = 0.876$ at. units, $A = 1.8$ at. units, $\beta' = 0$ when $r = 2.6$ at. units) at distances of more than 4 at. units or energies less than 10^{-2} at. units are shown in Fig. 3, together with points corresponding to the repulsive energy (inversely proportional to $r^{7.25}$) obtained in [23] from an analysis of experimental data on the scattering of Hg atomic beams in helium. The coincidence with the theoretical curve of φ_{exch} is good.

Another curve in Fig. 3 shows the interaction energy of mercury and helium atoms, taking account of the dispersional attraction

$$\varphi(r) = \varphi_{\text{обм}}(r) - C_6^{\text{Hg–He}}r^{-6}, \tag{8}$$

where the Van der Waals constant $C_6^{\text{Hg–He}} = 14$ at. units [18]. However, at moderate and short distances, the dispersional attraction is considerably weakened [24, 25]. The reduction in attractive energy (the energy differences calculated when the configurational interaction is disregarded and taken into account) in comparison with the energy $C_6^{\text{Na–Ar}}r^{-6}$ for Na–Ar interaction [3] is evident from Fig. 1. In a rough calculation, the curve of the attractive energy $\varphi_{\text{at}}^{\text{M–G}}(r)$ of atoms of particular metals and gases may be plotted using the approximate conversion relation

TABLE 2. Values of PD_{12} and n Calculated from Asymptotic Theory for Mixtures of Two-Electron Metals with Helium and Argon

Mixture	T_{ref}, K	PD_{12}, N·sec⁻¹	d_1	n	n^{gen}
Hg—He	470	13,1	0,94	1,77	1,75
		(14,1)	1,2	1,79	
		{13,0}	0,94	1,77	
Cd—He	780	{29,0}	1,21	1,81	1,75
Zn—He	890	{38,3}	1,04	1,81	1,75
Hg—Ar	470	3,5	1,16	1,73	1,75
Hg—Ne	470	6,1	0,72	1,74	1,75

Note. Figures without parentheses correspond to $\varphi(r)$ defined from Eq. (10), those with parentheses to $\varphi(r)$ from Eq. (8), and those with curly brackets to $\varphi(r) = \varphi_{\mathrm{exch}}(r)$; d_1 is the ratio of theoretical and experimental values of PD_{12}.

$$\varphi_{\mathrm{at}}^{\mathrm{M\text{-}G}}(r) = \varphi_{\mathrm{at}}^{\mathrm{Na-Ar}}(r)\, C_6^{\mathrm{M\text{-}G}} / C_6^{\mathrm{Na-Ar}}, \tag{9}$$

where the subscript M-G denotes the corresponding metal and inert gas (like the superscript Na—Ar; for this pair of atoms, $C_6^{\mathrm{Na-Ar}} = 190$ at. units [18]). Then

$$\varphi(r) = \varphi_{\mathrm{exch}}(r) - \varphi_{\mathrm{at}}^{\mathrm{M\text{-}G}}(r). \tag{10}$$

For Hg—He, the curve of $\varphi(r)$ plotted using Eq. (10) is also known in Fig. 3a. Calculation by Eq. (8) or (10) for large distances shows that the depth of the attractive potential well is very small for Hg—He (less than 10°K). Hence, the approximation in Eq. (2) may also be used in calculating the diffusion coefficient in this case.

The results of calculating PD_{12} for Hg—He for the reference temperature T_{ref} are shown in Table 2, together with the values of the exponent n for the temperature range 300-2000°K. Calculations are performed with $\varphi(r)$ defined by Eq. (10) and by Eq. (8), and also under the assumption $\varphi(r) = \varphi_{\mathrm{exch}}(r)$. The difference in the values of PD_{12} is not very large. The theoretical values of PD_{12} are compared with the mean experimental values, which are below those calculated from the generalization by a factor of 1.08 (therefore, the comparison with experimental data is more revealing; remember that the accuracy of the generalization is around ±10%). The agreement is found to be satisfactory. Table 2 also gives values of n^{gen}, which do not differ greatly from n, i.e., it is unnecessary to introduce corrections of the type of Eq. (3).

As well as theoretical results for Hg—He, Table 2 gives analogous results for the mixtures Zn—He and Cd—He (for Zn, $\beta = 0.831$ at. units, $A = 1.69$ at. units; for Cd, $\beta = 0.813$ at. units, $A = 1.6$ at. units). Values of the constant C_6 for the given pairs of atoms are not given in the literature. Therefore, calculations are performed only under the assumption that $\varphi(r) = \varphi_{\mathrm{exch}}(r)$. There is sufficient agreement between the theoretical and experimental values of PD_{12} [26, 27]. In the case of Cd—He, the agreement improves as the asymptotic coefficient A increases. If, for example, $A = 1.8$ at. units is taken, the ratio of the theoretical and experimental values of PD_{12} decreases to 1.15.

In [27], values of PD_{12} were determined on a specially developed high-temperature apparatus (by the Stefan method) both for Cd—He mixtures and for mixtures with argon and molecular nitrogen in the temperature range 670-970°K. Recently, on the same apparatus, there have been measurements of PD_{12} for Mg—He mixtures in the temperature range 770-1170°K, also corresponding to the generalization of [11].

Note also that satisfactory agreement between the theoretical and experimental values of PD_{12} for Hg—Ar and Hg—Ne may be obtained if Eq. (6) with a finite ρ is used for φ_{exch}. The electron scattering length at the argon atom is $L = -1.6$ at. units [19]. Taking $\rho = 3.1$ at. units, the value of φ_{exch} calculated from Eq. (6) corresponds both to the value obtained in [3] (disregarding configurational interaction) for Na—Ar (Fig. 1) and the value of the repulsive energy of Hg—Ar obtained from the data on the scattering of a Hg atomic beam in argon [23] (Fig. 3b). When using Eq. (10) for $\varphi(r)$ in calculating PD_{12}, the value in Table 2 is obtained for Hg—Ar. It does not differ greatly from the experimental value [11]. The agreement of the results calculated for PD_{12} and those found from the generalization of [11] for Hg—Ne is somewhat worse (there are no experimental data for this mixture) if $\rho = 1.1$ at. units is assumed in the analogous calculations together with $L = 0.2$ at. units according to

[19]. Calculations using data in the scattering of Hg atoms in Ne lead to a still lower value of PD_{12}. The values of ρ for helium, neon, and argon assumed in the calculations depend linearly on the ionization energy of the gas.

There also exist data on the repulsive energy for Hg—Kr and Hg—Xe [23]. However, calculation of φ_{exch} for these mixtures involves introducing excessively large values of ρ, comparable with the internuclear distances, since the heavy inert gas is characterized by large negative values of the electron scattering length (for krypton, $L = -3.2$ at. units; for xenon, $L = -5.8$ at. units [19]). Evidently, other calculation methods are needed for such cases.

NOTATION

$\varphi(r)$, potential energy of atomic interaction, depending on the distance between the nuclei r, at. units; P, total pressure in the binary gas mixture, Pa; D_{12}, mutual-diffusion coefficients of the components in the binary gas mixture, m^2/sec; T, absolute temperature, °K; M_1 and M_2, atomic masses of the components, kg/kmole; $Q_{12}^{(1,1)}$, mean diffusional cross section, $Å^2$; φ_{exch}, potential energy of the exchange interaction of the metal atom and the gas atom, at. units; $\beta = \sqrt{2 \cdot I_1}$, I_1, ionization energy (single ionization) of the metal atom, at. units; L, electron scattering length at an inert-gas atom, at. units; I(r), asymptotic wave function of the valence electron of the unperturbed metal atom,; A, asymptotic coefficient, at. units; α_2, polarizability of the inert gas, at. units.

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DETERMINATION OF COEFFICIENT OF THERMAL EXPANSION FOR BINARY COMPOSITE MATERIALS

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The coefficient of thermal expansion is determined for two-phase materials on the basis of the percolation model.

1. Structural Model of Nonhomogeneous Material. The analysis of heat conduction and electrical conduction in binary heterogeneous materials with random distribution of equipollent components is usually based on the percolation theory (theory of flow-through) [1, 2]. One of the main applications of this theory is determining the topology of an infinite cluster or, in other words, the distribution of components in such material as their volume concentration changes. It has been established [1, 2] that as the volume concentration v_1 of the first component in a continuous binder changes over the $0 \leqslant v_1 \leqslant v_c$ range (v_c is the percolation threshold), there appear isolated inclusions (insular clusters) of the first component and with $v_c \leq v_1$ bonds develop between them which transforms these insular clusters into infinite ones, this jumpwise transition occurring at the concentration $v_1 = v_c$ and being followed by formation of two equipollent infinite clusters when $v_1 \simeq v_2 \simeq 0.5$ in the material. A further increase of the volume concentration of the first component $v_1 > 0.5$ results in a structural reversal, namely an infinite cluster of the second component will decrease and at the concentration $v_2 = v_c$ be jumpwise transformed into an insular one while an infinite cluster of the first component continues growing.

Using the concepts of the percolation theory and the methods of reduction to an elementary cell, a structural model of a heterogeneous material has been proposed [3, 4], an elementary cell of which is shown here in Fig. 1. The geometrical parameters of such an elementary cell are given in Table 1. On the basis of this model theoretical relations for the effective thermal and electrical conductivities which agree closely with experimental data [3, 4] have then been derived.

Now, using this percolation model, we will determine the coefficient of thermal expansion for a heterogeneous material.

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