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High Temperature, Vol. 37, No. 1, 1999, pp. 45–51. Translated from Teplofizika Vysokikh Temperatur, Vol. 37, No. 1, 1999, pp. 49–55.

THERMOPHYSICAL PROPERTIES OF MATERIALS

Analytical Representation of Collision Integrals for the (*m*–6) Lennard–Jones Potentials in the EPIDIF Database

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Received December 19, 1997

Abstract—Based on the requirements of the EPIDIF database as regards the interaction potentials and the diffusion coefficients of species of gas-phase epitaxy of novel materials, the choice is justified of the set of the collision integrals, of the range of reduced temperatures, and of the desired accuracy of approximation of tabulated data. For the set of three-parameter m–6 Lennard–Jones potentials, the main collision integrals are approximated in the range of reduced temperatures $T^* = 0.4$–200 and, for the first time, in almost the entire range of the exponent $m = 8$–∞ with the standard deviation of 0.075–0.085%. The models and their parameters are introduced to the EPIDIF database and used to analyze the surface of the binary diffusion coefficient as a function of the variables T^* and m.

The development of databases in the transport properties of rarefied gases and their mixtures involves the problem of convenient representation of the collision integrals used to express appropriate kinetic coefficients in molecular physics [1, 2]. Obviously, every database, in accordance with its subject and objectives, imposes special demands on the completeness, authenticity, and other features of the input data. Our purpose was to satisfy the requirements of the EPIDIF database with respect to interdiffusion of the species of gas-phase epitaxy of semiconductor materials. This database is installed at the Institute of High Temperatures of the Russian Academy of Sciences as a part of the federal program on new materials. At the same time, we had in mind the problem of obtaining numerical data for the calculation of the transport properties of the combustion products of organic fuels.

The special features of the EPIDIF database are as follows.

(1) There is a great diversity of initial gaseous reagents such as hydrides, halides, and metal-organic compounds, which are used in chemical vapor deposition (CVD) process for epitaxially growing various semiconductors (Si, GaAs), isolators (Al_2O_3, SiO_2), and metal bondings (W, Mo, Pt) on the solid surface of a given structure [3]. The vapors of the reagents are transported into the reaction zone with the aid of carrier gases H_2, He, N_2, etc.

(2) The CVD processes are usually performed at a pressure from 1 to 10^3 mm Hg and at a temperature from 500 to 2000 K, i.e., in the range of states, in which the models of binary collisions of particles are valid for the gas phase with high precision.

(3) In simulating the processes of gas-phase epitaxy, the equations of gas dynamics and heat and mass transfer for the species and for the reacting mixture as a whole are treated simultaneously [4, 5]. For solving them, one must know, in particular, the diffusion coefficients, the coefficients of thermal diffusion of the species, as well as viscosity and thermal conductivity of the mixture. The natural basis for calculating a complete and consistent system of kinetic coefficients is provided by the modern apparatus of molecular kinetic theory of rarefied gases [1, 2] and by pair potentials of interparticle interactions, which are used to compute the respective integrals in the kinetic theory.

The diverse species involved in CVD processes are characterized, from the standpoint of types of interaction, by different potentials ranging from central-symmetrical potentials for atoms and quasi-spherical molecules (SiH_4, WF_6) to complex nonspherical potentials for dipole molecules (HF, HCl, AsH_3, etc.). Taking into account the great number of the species and the mass character of operations in the EPIDIF database, we did not consider it possible to perform the computation of the kinetic coefficients on the basis of individual multiparameter potentials presently known for inert gases [6]. At the same time, the simplest two-parameter 12–6 Lennard–Jones potential (L–J 12–6) widely used for the calculation of properties of gases [1, 7–9] is not flexible enough. In particular, this potential fails to convey the soft repulsion of the particles of the carrier gases in the CVD processes such as He [10] and H_2 [11]. At the same time, this potential fails to provide the high rigidity that is necessary for the description of the properties of globular molecules such as SF_6 and WF_6 [12].

As a result of analysis of three-parameter potentials of different types [13], we chose the set of inverse-power L–J (*m–6*) potentials (with the parameters ε—the depth of the potential well, d—the collision diameter, and m—the exponent of the repulsion branch). We made this choice in view of the following.

(1) For these potentials in a wide range of reduced temperatures $T^* = T/\varepsilon = 0.1–200$ and exponents $m = 8–75$, tabulated data on the classical collision integrals $\Omega^{(l,s)*}$ have been published, calculated with the accuracy better than 10^{-3} [14–17].

(2) By varying the exponent m, it is possible to describe the transport properties of a great number of gases that are typical of CVD processes with both soft ($m = 8–9$ [10, 11]) and hard ($m = 30–40$ [12]) repulsion.

(3) Finally, there exists preliminary experience of approximating the integrals $\Omega^{(1,1)*}$ and $\Omega^{(2,2)*}$ as functions of the variables T^* and m.

The operating range of reduced temperatures for the EPIDIF database is assumed to be $T^* = 0.4–200$. The upper boundary is estimated for helium (ε(He) ~ 10 K) and the maximum temperature of CDV processes $T_{\max} = 2000$ K. The estimation of the lower boundary is based on the presence in the database of species with high values of $\varepsilon = 800–1000$ K (e.g., Hg) and $T_{\min} = 500$ K.

The accuracy of modern precision measurements of the viscosity and diffusion coefficients of gases [2] is not worse than 0.3–0.4%. Taking this into account, we assumed that the calculation error for the collision integrals in the EPIDIF database must be 2×10^{-3} or less.

For the light pair H_2–CH_4, the de Boer quantum parameter is $\Lambda^* = h/(d_{12}\sqrt{2\mu\varepsilon_{12}}) \simeq 1$, where h is the Planck constant and μ is the reduced mass. In this case, the upper estimate for the quantum correction to the classical integrals $\Omega^{(l,s)*}$ at $T = 500$ K [1, 17] does not exceed $(1.5–2) \times 10^{-3}$, which gives grounds for the use of the classical collision integrals in the database.

Based on the results of analysis of the relations of the molecular kinetic theory [1, 2], we chose the set of integrals $\Omega^{(1,1)*}$, $\Omega^{(1,2)*}$, $\Omega^{(1,3)*}$, $\Omega^{(2,2)*}$, and $\Omega^{(2,3)*}$ or the equivalent set of the coefficients $\Omega^{(1,1)*}$, $C^* = \Omega^{(1,2)*}/\Omega^{(1,1)*}$, $B^* = (5\Omega^{(1,2)*} - 4\Omega^{(1,3)*}/\Omega^{(1,1)*} = 1 + 3C^* - 3C^{*2} - (T^{*2}/3)(\partial^2 \ln\Omega^{(1,1)*}/\partial T^{*2})$, $\Omega^{(2,2)*}$, and $E^* = \Omega^{(2,3)*}/\Omega^{(2,2)*}$ to be represented in the EPIDIF database. This set is sufficient for the computation of the kinetic coefficients for pure gases in the second approximation of the theory, for the diffusion coefficients of species of the mixture in the second approximation, and for the coefficient of thermal diffusion in the first approximation. The results of calculation of the diffusion coefficient of a species in a mixture of gases of sharply differing masses (H_2–N_2–Xe, Ne–Ar–Kr) reveal that the difference in the coefficients computed in the third and second approximations ($[D_{ij}]_3/[D_{ij}]_2 - 1$) at $T = 300$ K is less than 10^{-3} [19].

Therefore, the requirements of a concrete database with regard to the kinetic coefficients permit one to define the necessary set of collision integrals, the accuracy of representation, the range of reduced temperature, and, finally, some set of the potential functions.

The L–J (*m–6*) function is written in two ways, namely, as a function of $X = r/r_e$, where r_e is the equilibrium distance, $U(X = 1) = -\varepsilon$, and $(\partial U/\partial X)_{X=1} = 0$, or as a function of $R = r/d$, where $U(R = 1) = 0$ (at $U(R \longrightarrow \infty) \longrightarrow 0$). For example,

$$U/\varepsilon = U^* = [(m/(m-6))(m/6)^{6/(m-6)}](R^{-m} - R^{-6}). \quad (1)$$

The exponent m is an empirical quantity and may vary continuously within $m = 6–\infty$ [2, 20]. At $m \longrightarrow \infty$, relation (1) degenerates to the Sutherland potential [1]. The curvature of function (1) at its minimum is $p = (\partial^2 U^*/\partial X^2)_{X=1} = 6m$. By varying the value of m, it is possible to change in a wide range both the slope of the repulsion branch and the curvature at the minimum. At $m = 10$, we have $p = 60$, which is much closer to the experimental data for inert gases than the value of 72 obtained for the L–J (12–6) potential.

We treated several alternative versions of the representation of the collision integrals $\Omega^{(l,s)*}(T^*, m)$ in the database for preassigned potentials (1), in particular, the possibility of computation using conventional software packages [2, appendix *A*; 21, 22], the input of two-dimensional tabulated data on $\Omega^{(l,s)*}(T^*, m)$ [14–16], and, finally, their approximation by parametric dependences $\omega^{(l,s)*}(T^*, m, \mathbf{a})$. The last approach has been chosen because it provides wider opportunities for independent users.

Numerous attempts to approximate collision integrals in a wide range of temperatures were made previously, mainly for the L–J (12–6) potential [18, 23–26]. In choosing the type of the dependence $\omega_m^{(1,s)*}(T^*, \mathbf{a})$, it is customary to assume that the importance of the attraction branch of the potential at high temperature may be ignored and that the process of collision is completely due to the repulsion forces. In contrast, it is assumed that, at $T^* \ll 1$, the attraction forces play the dominant role.

For monotonic inverse-power potentials, the following equation is known:

$$\Omega_{+,-}^{(l,s)*} \sim (m/T^*)^{2/m}\Gamma(s + 2 - 2/m)A_{+,-}^{(l)}(m), \quad (2)$$

where m is the exponent; Γ is the gamma-function; and the coefficients $A^{(l)}(m)$ are calculated at $l = 1–4$ (1) and $m = 2–\infty$ for both attractive A_+ and repulsive A_- potentials [1, 27].

Equation (2) gives ground to expect that $\omega^{(l,s)*} \sim T^{*\,-1/6}$ potential and $T^* \gg 1$ and $\omega^{(l,s)*} \sim T^{*\,-1/3}$ at $T^* \ll 1$ (i.e., in the classical limit). It is these asymptotics that are used in the models [18, 23–25] in some or other form. Note that it is possible to describe the collision integrals in the temperature range $T^* = 3–200$ with the accuracy of about 2% by the dependences of the type of $\omega^{(l,s)*} \sim T^{*-1/b}$, and this fact is often used to represent the integrals at moderate and high temperatures [7].

Expressions have gained acceptance that approximate the tables of sixteen integrals for the L–J (12–6) potential, which are refined with respect to [1], in the range $T^* = 0.3$–400 with the accuracy better than 10^{-3} [25],

$$\omega^{(l,s)*} = AT^{*-\mathbf{B}} + \sum_{1}^{3} a_i \exp(-b_i T^*) + RT^{*B}\sin(ST^{*W} - P), \quad (3)$$

where each (l, s) is assigned its parameters, and $\mathbf{B} = 0.152 \pm 0.004$. The exponential terms introduce a correction for attraction to the repulsion core $A/T^{*\mathbf{B}}$. The last term in (3) is intended to compensate for typical wavelike deviations that occur during "nonstatistical" approximation of smooth tables.

Fokin *et al.* [18] successfully performed separate approximation of the tabulated data on $1/\Omega^{(1,1)*}$ and $1/\Omega^{(2,2)*}$ on the isolines of $m = \text{const}$ ($m = 9$–15 (1)) in the range $T^* = 0.2$–30 by the method of least squares. Fractional rational functions were used, which joined the low-temperature $1/\Omega^{(l,s)*} \sim T^{*1/3}$ and high-temperature $1/\Omega^{(l,s)*} \sim T^{*1/6}$ asymptotics (2) of the integrals for the L–J (12–6) potential. The parameters of the model were found using the quasi-linearization procedure described by Spiridonov [28].

It is interesting to treat the model [29], which employs switching functions of the type $[(1 + T^*/B)^{\beta}]^{-1}$ and $[(1 + B/T^*)^{\beta}]^{-1}$. These functions join the low- and high-temperature asymptotics of collision integrals (2). The results of approximation of the isolines of $\Omega^{(1,1)*}$ and $\Omega^{(2,2)*}$ from [2] at $m = 9, 12, 18$ in the range $T^* = 0.1$–100 with the accuracy of about 0.5–0.9% are given in [29].

The examples of two-dimensional approximation of $\Omega^{(l,s)*}(T^*, m)$ are not numerous.

Previously, a short expansion of the integrals $\Omega^{(1,1)*}$ and $\Omega^{(2,2)*}$ into the Taylor series relative to $m = 12$ in a narrow region of variation of the exponent $m = 12 \pm 3$ was used in the β-version of the EPIDIF database [30].

The $\Omega^{(2,2)*}(T^*)$ isolines in the range $T^* = 0.3$–10 for $m = 9$–18 (1) were described in [18] by the dependences of type $\omega^{(2,2)*} = -b_k \ln T^* + \sum_1^4 a_i T^{*(1-i)}$, and then the parameters $b(m)$ and $a_i(m)$ were approximated by polynomials in powers of $1/m$.

We used the accumulated experience [18, 23–26, 29–30] in view of the foregoing requirements of the EPIDIF database to perform a two-dimensional approximation of the tabulated data on the collision integrals $\Omega^{(1,1)*}$ and $\Omega^{(2,2)*}$ [14–16] in the ranges of temperature $T^* = 0.4$–200 and exponents $m = 8$–∞ using expressions of the $(k = 1, 2)$ form,

$$\ln\omega^{(k,k)*} = -\frac{2}{m}\ln T^* + \delta^{(k,k)}\ln\left(1 - \frac{2}{3m}\right) + \sum_{i=1}^{P} a_i^{(k,k)}(m)(1/T^*)^{(i-1)\Delta^{(k,k)}}, \quad (4)$$

where the coefficients $a_i(m)$, in their turn, had the form

$$a_i(m) = a_{i1} + a_{i2}/m + a_{i3}/m^2 + a_{i4}/m^3. \quad (4a)$$

In view of the special features of equation (2), it is assumed that $\delta^{(1,1)} \equiv 0$ and $\delta^{(2,2)} \equiv 1$. Relations (4) and (4a) include the empirical correction for the forces of attraction to the collision integrals of the repulsion branch of the L–J (*m*–*6*) potential. At $T^* \longrightarrow \infty$, we have $C^* \longrightarrow 1 - 2/(3m)$ and $B^* \longrightarrow 1 + 4/(3m) - 4/(3m^2)$.

Because the L–J (*m*–*6*) potential degenerates to the Sutherland potential at $m \longrightarrow \infty$, for whose collision integrals the high-temperature expansion has the form $\Omega^{(l,s)*} \sim 1 + S/T^*$, we arrive at $a_{11}^{(1,1)} \equiv a_{11}^{(2,2)} \equiv 0$ in (4) and (4a).

The approximation by expressions (4) and (4a) to the tabulated data was performed by parametric minimization of the following quadratic functional:

$$\begin{aligned} S &= \Sigma W_{1i}[\ln\Omega_i^{(1,1)*}(T^*, m) \\ &\quad - \ln n\omega_i^{(1,1)*}(T^*, m, \mathbf{a}^{(1,1)})]^2 \\ &\quad + \Sigma W_{Ci}[C_i^*(T^*, m) - c_i^*(T^*, m, \mathbf{a}^{(1,1)})]^2 \\ &\quad + \Sigma W_{2i}[\ln\Omega_i^{(2,2)*}(T^*, m) \\ &\quad - \ln n\omega_i^{(2,2)*}(T^*, m, \mathbf{a}^{(2,2)})]^2 \\ &\quad + \Sigma W_{Ei}[E_i^*(T^*, m) - e_i^*(T^*, m, \mathbf{a}^{(2,2)})]^2 \\ &\quad + \Sigma W_{Ai}[\ln A_i^*(T^*, m) \\ &\quad - \ln n\omega_i^{(2,2)*}(T^*, m, \mathbf{a}^{(2,2)}) \\ &\quad + \ln n\omega_i^{(1,1)*}(T^*, m, \mathbf{a}^{(1,1)})]^2. \end{aligned} \quad (5)$$

The coefficients C^* and E^* were found with the aid of the expression [1, 2]

$$\Omega^{(l,s+1)*}/\Omega^{(l,s)*} = 1 + (\partial\ln\Omega^{(l,s)*}/\partial\ln T^*)/(s+2) \quad (6)$$

by differentiating (4) and (4a) with respect to $\ln T^*$. In this case, the functions remain linearly dependent on the parameters $\mathbf{a}^{(k,k)}$.

In functional (5), a simultaneous approximation of functions (4), and their temperature derivatives is performed. This leads to the intrinsic consistency of the

Table 1. The results of approximation of collision integrals

No.	Tabulated data	Number of points	Functional	
			$S(a_{i-1} =$ const)	$S(a_i =$ var)
1	$\Omega^{(1,1)*}$	770	–	27.06
2	$+\Omega_s^{(1,1)*}$	796	36.89	30.05
3	$+C^*_{(9,12,50)}$	937	61.68	51.82
4	$+C^*_{(T^* = 0.4)}$	951	126.06	64.55
5	$\Omega^{(2,2)*}$	770	–	68.67
6	$+\Omega_s^{(2,2)*}$	797	84.16	80.87
7	$+E^*_{(9,12,50)}$	938	110.16	104.85
8	$+E^*_{(T^* = 0.4)}$	952	218.48	131.71
9	$+\Omega^{(1,1)*} + C^* +$ $+\Omega^{(2,2)*} + E^*$	1903	296.25	196.25
10	$+A^*_{(9,12,50)}$	2044	201.49	201.22
11	$+A^*_{(T^* = 0.4)}$	2058	202.20	201.92

integrals $\omega^{(1,1)*}$ and $\omega^{(1,2)*}$, on the one hand, and of $\omega^{(2,2)*}$ and $\omega^{(2,3)*}$, on the other hand. Functional (5) includes the coefficient $A^* = \Omega^{(2,2)*}/\Omega^{(1,1)*}$, which is used, in particular, to compute the diffusion coefficient in the second approximation of the theory.

The statistical weights are supposed to be $W_i = \Delta_i^{-2} = (2 \times 10^{-3})^{-2}$ for all tabulated values in (5) with the exception of those for the Sutherland potential. Certain difficulties arise in the application of the tabulated data for $\Omega_s^{(1,1)*}$ and $\Omega_s^{(2,2)*}$ for the Sutherland potential [1] calculated by Kotani in 1941 [31]. The results of analysis at $T^* > 2$ demonstrate that the isotherms $\Omega^{(l,s)*} = f(1/m)$ at $m = 8$–75 in [14–16] as functions of $1/m$ and extrapolated to zero agree naturally with the integrals from [31]. However, at $T^* < 1.5$, a discrepancy occurs, and at $T^* = 0.4$ the difference $\Omega^{(1,1)*}(m \longrightarrow \infty) - \Omega^{(1,1)*}$ [31] reaches 1.5%.

The problem of extrapolation of the isotherms of high-temperature collision integrals to $m \longrightarrow \infty$ is discussed in [32]. It is at low temperatures $T^* < 1.5$ that the observed disagreement occurs and the reason for this is as yet unknown. That is why we performed the approximation using the integrals given in [31] at $T^* = 0.25$–1.33 with the accuracy of 4–0.4% and further at $T^* > 1.5$ with the accuracy of 0.2%. The tables of the coefficients C^*, E^*, and A^* [14–16] with all fourteen values of m on the isotherm $T^* = 0.4$ are also included in the data processing. The number of points in the array $\langle \Omega^{(1,1)*} - C^* \rangle$ is 952, and that in the array $\langle \Omega^{(2,2)*} + E^* \rangle$ is 953. The total number of points including the data for the coefficient A^* is 2058.

The parameters of model (4) and (4a) were found with the aid of the FUMILI package [33], which is the FORTRAN version of the least squares method, with the double precision representation of the data.

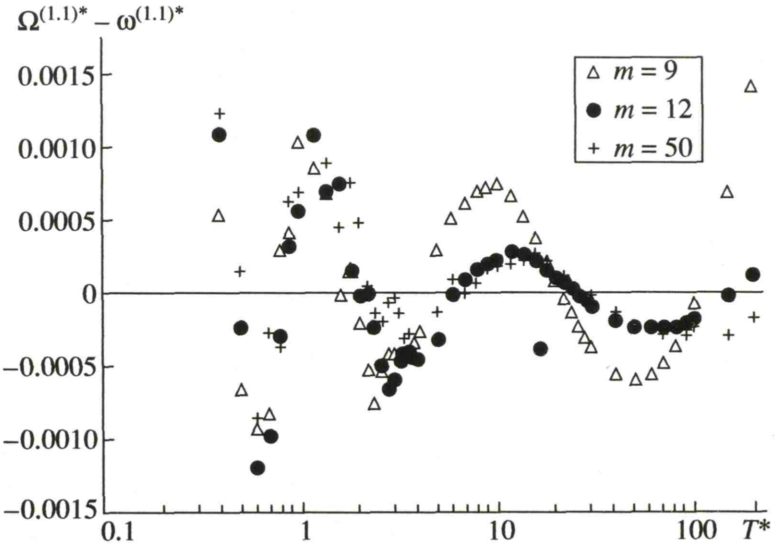
An adequate agreement between model (4) and (4a) and the tabulated data discussed above is obtained with the number of about 20–24 for each of the parameters $\mathbf{a}^{(1,1)}$ and $\mathbf{a}^{(2,2)}$. In so doing, the standard deviation in the data array $\langle \Omega^{(1,1)*} + C^* \rangle$ is about 0.07%, and in the array $\langle \Omega^{(2,2)*} + E^* \rangle$ it is about 0.085%. The deviations of the calculated values from tabulated ones on the m-isolines have a typical wavelike form. The deviations in the former array are less than 0.2% in all cases except for the low-temperature points [31], and in the latter array they may be as great as 0.25%, especially at $T^* = 0.4$–0.6.

The optimal values of two nonlinear parameters $\Delta^{(k,k)}$ in (4) were determined at minimization (5) by the trial-and-error method for each data array. These values turned out to be in the range of 0.5 ± 0.02. To facilitate the calculation, we assumed $\Delta^{(1,1)} = \Delta^{(2,2)} = 0.5$. The details of the calculation and the values of the respective parameters are given in [34].

Note that the coefficients B^*, which were not involved in the approximation procedure and the calculation of which involves second-order derivatives, can be found by (4) and (4a) with an error of less than 0.5%.

In the implementation of the least squares method [33] in a preset data array, the functional was observed to decrease monotonically with the increase of the number of parameters. This is evidence of an insignificant effect of the calculation errors, particularly, in the matrix inversion procedure performed by the FUMILI package. Nevertheless, we performed independent computations by computer codes based on the use of the least squares method [35], adapted to multidigit arithmetic software [36] in order to quantitatively estimate the calculation errors in the parameters of model (4) and (4a). In doing so, we used the "standard" array of the integrals $\langle \Omega^{(1,1)*} + \Omega_s^{(1,1)*} \rangle$ [14–16, 31] in the range of $T^* = 0.4$–200 and $m = 8$–∞ with the statistical weights as given above. The array contained 796 points.

The package [35] includes the procedures of transformation of the initial system of the least-squares equations to the orthogonal decomposition basis. The orthogonalization was performed using recurrent expressions enabling one to efficiently use the computer memory, which is especially important for the memory-intensive package of multidigit arithmetic [36]. The computation was carried out with the data representation with 42 digits. During the approximation of the "standard" data array in a model character-



Deviation of the tabulated integrals $\Omega^{(1,\,1)*}$ from the calculated ones $\omega^{(1,\,1)*}$.

ized by 24 parameters ($a_{11} \equiv 0$), the divergence of the coefficients calculated previously by the FUMILI package and the coefficients produced by the package of [35] did not exceed unity in the fifth order of decimal mantissa. This difference is negligible with the preassigned computation accuracy of the collision integrals. The increase from 24 to 46 of the number of the parameters in model (4) and (4a) used for the approximation in the regime of multidigit arithmetic results in a monotonic decrease of the functional from $S_{24} = 55.17$ to $S_{46} = 10.08$.

The employed model (4) and (4a) is in fact an expansion in powers of $(1/T^*)$ and $(1/m)$ of the term correcting for the attraction to the integrals for the repulsion potential (2). On the other hand, one can see from (2) (see also [32]) that the dependence $\ln\Omega^{(l,\,s)*} = f(m)$ may include terms of the form $(1/m)\ln(1/m)$. The possibility is studied of the representation of the coefficients $a_i(m)$ in (4) in the form

$$a_i(m) = a_{i1} + a_{i2}/m + a_{i3}/m^2 + (a_{i4}/m^2)\ln(1/m). \quad (4b)$$

This results in a 1.5-fold decrease of the functional S of the array of $\langle\Omega^{(1,\,1)*} + \Omega_s^{(1,\,1)*}\rangle$ in comparison with the initial functional used in model (4) and (4a) [34]. The version of the model (4) and (4b) is used below. Table 1 shows the dynamics of variation of the functional at constant increments of the data arrays. One can clearly see the advantages of the procedure involving the simultaneous approximation of the function and its derivative (see the arrays $\langle\Omega^{(1,\,1)*} + C^*\rangle$ and $\langle\Omega^{(2,\,2)*} + E^*\rangle$, respectively).

For formal reasons, one parameter of the vector $\mathbf{a}^{(1,\,1)}$ and three parameters of $\mathbf{a}^{(2,\,2)}$ are additionally assumed to be insignificant in the final version (4) and (4b). The values of the coefficients for the functional $S = 201.97$, rounded off to six significant digits, are given in Table 2.

Table 2. The parameters of approximating expressions (4) and (4b), $\Delta^{(1,1)} = \Delta^{(2,2)} = 0.5$

$a^{(k,\,k)}$	$k = (1,1)$	$k = (2,2)$	$a^{(k,\,k)}$	$k = (1,1)$	$k = (2,2)$
a_{11}	0	0	a_{41}	0.485352	0.697682
a_{12}	-0.145269×10	0.113086×10	a_{42}	0.245523×10^2	0.590192×10^2
a_{13}	0.294682×10^2	0.234799×10^2	a_{43}	-0.336782×10^3	-0.143670×10^3
a_{14}	0.242508×10	0.310127×10	a_{44}	0.814187×10^2	-0.123518×10^3
a_{21}	0.107782×10^{-1}	0	a_{51}	-0.385355	-0.564238
a_{22}	0.587725	0.551559×10	a_{52}	-0.206868×10^2	-0.430549×10^2
a_{23}	-0.180714×10^3	-0.137023×10^3	a_{53}	0.132246×10^3	0
a_{24}	0.595694×10^2	0.185848×10^2	a_{54}	0	0.137282×10^3
a_{31}	0.546646×10^{-1}	0.325909×10^{-1}	a_{61}	0.847232×10^{-1}	0.126508
a_{32}	-0.651465×10	-0.292925×10^2	a_{62}	0.521812×10	0.104273×10^2
a_{33}	0.374457×10^3	0.243741×10^3	a_{63}	-0.181140×10^2	0.150601×10^2
a_{34}	-0.137807×10^3	0	a_{64}	-0.747215×10	-0.408911×10^2

A typical graph of the deviations of the tabulated integrals $\Omega^{(1,1)*}$ from the calculated ones $\omega^{(1,1)*}$ on the isolines of $m = 9, 12, 50$ is given in the figure.

The resultant model is a convenient tool for the analysis of collision integrals and kinetic coefficients proper.

For example, the collision integrals $\Omega^{(1,1)*}(T^*, m)$ and $\Omega^{(2,2)*}(T^*, m)$ have a singular feature according to which the isolines of constant m intersect at close temperatures. It is easy to find, using expressions (4) and (4a), that for the integrals $\Omega^{(1,1)*}$ at $m = 6$–100 the region of the intersection of the curves is located at $T^* = 1.58 \pm 0.08$.

ACKNOWLEDGMENTS

We are grateful to A.P. Kalinin, A.V. Lyusternik, I.A. Sokolova, and M.S. Trakhtengerts for advice and assistance in our work.

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