КОНДЕНСАЦИЯЛАНҒАН КҮЙДІҢ ФИЗИКАСЫ
ФИЗИКА КОНДЕНСИРОВАННОГО СОСТОЯНИЯ
PHYSICS OF THE CONDENSED MATTER

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Recurrent relations for correlation functions

We have considered the basic problem of the mathematical description of the viscous motion of a metallic melt, accompanied by the overcoming of internal friction caused by the motion of the melt particles and the overcoming of the forces of their interaction. The novelty of the research is that the correlation functions of viscosity are justified from the point of view of the quantum-statistical method. The correlation between correlation functions and the radial distribution functions is established. Based on the cluster theory of melt flow, a relationship is established between the viscosity and the interatomic potential. The relationships found allow us to determine the mean values of any physical parameters, and also to represent the potential energy of the system as a sum of the energies of the pair interaction of the particles. Two-particle radial distribution functions are sufficient to determine the average values of physical parameters, in particular, the transfer coefficients of molten metals. Three or more orders of correlation functions can be taken into account by recurrence formulas.

Keywords: metal melt, the hydrodynamic equations, correlation functions, quantum potentials, the quantum-statistical, mathematical modeling, computer simulation, density functional.

The theory of the liquid state is not a simple section of the modern theory of metallurgical processes. If the structure of solids is studied at a sufficient level and as a result of studying their properties, a rich experimental material is obtained, and this material is analyzed from the point of view of quantum physics and chemistry, this can not be said about liquids and liquid metal systems in general. Despite these problems, research in this field is continuously expanding due to the development of liquid state physics, physical chemistry and the theory of metallurgical processes.

In this case, hydrodynamic studies of melts, taking into account the micro- and nanostructure of the molten systems, are of particular importance. The accumulated knowledge in these areas as a whole makes it possible to solve many problems associated with the theory of the molten state and, obviously, have a positive effect on the progress of liquid state physics, the theory of metallurgical processes and, of course, metallurgical technologies. These studies are of great importance, since to this day has not yet been developed not only the general theory of solid and liquid states, but also of gaseous and plasma states [1].

Scientific novelty of the work consists in developing more perfect models for studying molten systems cluster structure, as well as in making an algorithm of computing geometry, potential energy of interaction and atoms radial distribution function in them.

Aim of work – to analyze and investigate the possibilities of using a semi-empirical quantum-chemical method for construction of atoms radial distribution in melts. To develop an algorithm of numerical modeling by a method of molecular dynamics of structural and physical- and- chemical properties of melts.

For specific calculations, a detailed physico-mathematical apparatus is needed. We will use the methods of statistical physics. It should be noted that the greatest successes have been achieved in this direction in the works of M. Born, G. Green, J. Kirkwood, N.N. Bogolyubov and others. And the main task of such a statistical theory of liquids is to establish a relationship between the properties of molecules and the interatomic potential, as well as between the thermodynamic and kinetic properties of molten systems. When studying the properties of the melt, it is necessary to take into account the set of particles for which the averaging of the physical quantities is performed. As is known [2], in the case of a crystal it is possible to obtain, for example, information pertaining to a single dislocation, but one can not track the motion of one impurity atom. And in melts, due to the high mobility of its particles and due to the absence of long-range order (as in a crystal lattice), the closest environments of different atoms or molecules can differ quite strongly, both in the number of neighbors and in their spatial arrangement. Since it is not possible to follow the behavior of a single atom or group of atoms, the so-called clusters, the results of measurements of any melt properties turn out to be averaged over a large number of atoms. When a property is studied which does not depend on the angular orientation (in space) of the nearest neighbors of a given atom, then, when averaging over different atoms, such an orientation can not be reflected as a result of the measurement, so that only the total number of atoms located at a certain distance from of the given atom.

To describe this situation, we choose a spherical layer with an internal radius r and an outer R layer centered on the nucleus of an arbitrary particle of a simple melt (containing for simplicity only the atoms of one element). In this case, the average number of atoms in this spherical layer will be proportional to the volume of the layer $4\pi r^2 dr$ and is determined by the following relationship:

$$dn(r) = 4\pi r^2 dr R(r), \tag{1}$$

where $R(r)$ is the so-called pair function of the radial distribution.

The function $R(r)$ in terms of its physical meaning is the density of the number of particles, but not the average, but local with respect to some arbitrary atom chosen as the origin. In the case when the distance r is sufficiently large in comparison with the interatomic distance r_a, individual atoms may not experience the action of the central particle and, therefore, will be located independently of it. In this case, we must substitute in equation (1) instead $R(r)$ of the usual average density $R(r\to\infty) = R_0$. In the case when the distance from the center of a given atom is too small (less than the so-called atomic diameter), then no nucleus of the particle will fall into the spherical layer. The function $R(r)$ has an oscillating character at small distances r. It is this behavior that corresponds to the structure of the melt, since some ordering features inherent in the crystal from which the melt was formed should appear in them. Thus, there must exist a pre-important distance between nearest neighbors, analogous to the interatomic distance in the crystal, the average number of nearest neighbors, analogous to the coordination number in the lattice, and so on. The existence of ordering elements in the melt, which is ultimately due to the intrinsic volume of the molecules and the features of the interatomic potential, is determined by the term short-range order.

If we were to consider an ideal gas, then instead of an oscillating curve, the radial distribution function $R(r)$ would be constant and equal to the average density R_0, since the particles of an ideal gas do not interact and have zero intrinsic volume. For example, the radial distribution function for liquid tin is shown in Figure.

Note that in addition to the function $R(r)$ itself, the value is often considered:

$$\frac{dn(r)}{dr} = 4\pi r^2 R(r).$$

A parabola is a graph $4\pi R_0 r^2$ to which it asymptotically tends $\frac{dn}{dr}$ at large distances r. Vertical lines describe the case of a crystal when the distances between atoms are fixed, and the height of the line is proportional to the number of neighbors in the corresponding coordination sphere. These results can be represented (table 1) in such a way that when the crystal melts, the peaks are blurred, forming the oscillating function $\frac{dn}{dr}$ depicted in Figure.

The causes of oscillations at small distances can be treated as the most probable arrangement of atoms in melts with increasing r.

Earlier, we defined a pair function of the radial distribution $R(r)$ that describes the average location of the melt particles around some arbitrary atom. Now, this need to be generalized to the case when we are interested in the relative positions of the number of atoms. To do this, we choose a volume dV in the melt. Let the average number of particles in this atom be equal to $dn = R_0 dV$, where R_0 is the number density of particles (the number of particles per unit volume). If we assume that dV it is sufficiently small, it dn will be much less than unity. Because of this, the product $R_0 dV$ can be considered as the probability of detecting a melt particle in a volume dV : $dW_1 = R_0 dV_1$.

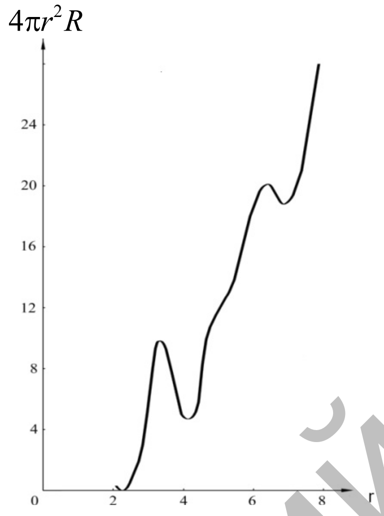

Figure. The curve of the atomic distribution for tin

Table

Curve of the atomic distribution for tin

r	2.1	2.3	2.5	3	3.5	4	4	5	5.3	5.5	6	6.5	7	7.5	8
$4\pi r^2 R$	0.3	0	0.5	5	9.8	6	5.8	11.5	12.7	13	18	20.1	18.8	21	28

Let us select in the melt the following volume elements dV_1 and dV_2 near points with radius vectors r_1, r_2. Let us determine the probability that in volumes dV_1 and dV_2 simultaneously there will be two particles. Then this probability should be proportional to the volumes themselves, that is:

$$dW_{12} = R_2(r_1, r_2) dV_1 dV_2, \tag{2}$$

where $R_2(r_1, r_2)-$ the function is the so-called binary correlation function.

If we assume that the volumes dV_1 and dV_2 are far from each other, then the probabilities of particles entering these volumes become independent and, by the theorem on multiplication of probabilities, we can write:

$$dW_{12} = dW_1 dW_2 = R_0^2 dV_1 dV_2.$$

It can be seen from the relations (2) that for large values of $|r_1 - r_2|$ it follows that $R_2(r_1, r_2) = R_0^2.$, similarly to what was said above, we can introduce the probability $dW_{1,2,\ldots,n}$ that there will be one particle in the volumes $dV_1, dV_2, \ldots, dV_n$. Define $dW_{1,2,\ldots,n}$ it as follows:

$$dW_{1,2,\ldots,n} = R_n(r_1, r_2, \ldots, r_n) dV_1 dV_2 \ldots dV_n. \tag{3}$$

The function of the coordinates of all $n-$ particles R_n introduced by Eq. (3) is called the correlation function of the n order. As before, as the distance between each two volumes increases, the probabilities of finding particles in each volume become independent, that is, when it is obvious $|r_i - r_k|$ that It is necessary $R_1 \equiv R_0$. To emphasize that a particular case of a correlation function of the n order is the so-called ternary correlation function $R_3(r_1, r_2, r_3)$.

In addition, we can establish a connection between the binary correlation function and the pair function $R(r)$ of the radial distribution. The probability of finding two particles in volumes dV_1 and dV_2 can be represented as a product of two probabilities: first, that there is one particle dW_1 in the volume dV_1 and, secondly, that the second particle dW_2 is at a distance $|r_1 - r_2|$ from the first particle. Thus, dW_2 this is the probability of the second event, provided that the first has already occurred:

$$dW_2 = R(|r_2 - r_1|)dV_2.$$

The probabilities dW can be normalized as follows:

$$\int dW_1 = \int_V R_0 dV_1 = R_0 V = N,$$

where N is the total number of melt particles.

$$\int dW_2 = \int R_2(r_1, r_2) dV_1 dV_2 = N(N-1),$$

and correspondingly:

$$dW_n = \frac{N!}{(N-n)!}.$$

In practice, for convenience of calculations, it is expedient to reformulate the correlation functions and probabilities so that the former become dimensionless and that the norm integrals are equal to unity. To this end, we introduce new probabilities for a given configuration of n-particles of the melt:

$$dW_n = \frac{1}{V^n} F_n(r_1, r_2, ..., r_n) dV_1 dV_2 ... dV_n, \tag{4}$$

where $dV_i = dx_i dy_i dz_i$, x_i, y_i, z_i are the coordinates of that particle.

Naturally, the correlation function defined in this way is dimensionless. Further, it will be possible to require that the new probability be normalized to unity $\int dW_n = 1,$, that is,

$$\frac{1}{V^n} \int F_n(r_1, r_2, ..., r_n) dV_1 dV_2 ... dV_n = 1. \tag{5}$$

From equations (4) and (5) it is clear that:

$$d\omega_n = \frac{N!}{(N-n)!} dW_n.$$

The last equation suggests a reliable interpretation of probabilities $d\omega_n$. Probability dW_n refers to a given volume configuration, when it is not essential which particles occupy these volumes $dV_1, dV_2, ..., dV_n$. The volume dV_1 refers to any of the N particles, and the volume dV_2 refers to any of the remaining particles $N-1$, and so on. In view of this, an additional multiplier appears $\frac{N!}{(N-n)!}$. Taking into account relations (3) and (5), we find the correlation between the correlation functions R_n and F_n:

$$R_n(r_1, r_2, ..., r_n) = \frac{N!}{(N-n)!} \frac{1}{V^n} F_n(r_1, r_2, ..., r_n). \tag{6}$$

We note that the correlation functions of the two successive orders are related to each other by the relation (6), which follows from the definition of probability [3]. We now introduce the total potential energy of the system, which depends on the coordinates of all the melt particles. Because of this, according to Boltzmann-Gibbs statistics, the probability of this particle configuration is proportional to the factor $\exp\left[-\frac{U}{kT}\right]$.

Then:

$$dW_n = A \exp\left[-\frac{U(r_1, r_2, ..., r_n)}{kT}\right] dV_1 dV_2 ... dV_n.$$

Thus, the correlation function F_N can be determined from the potential energy of the system. Then we can construct recurrence relations for which allow us to find correlation functions F_N of lower orders:

$$F_N\left(r_1,r_2,...,r_n\right)=V^N A\exp\left[-\frac{U\left(r_1,r_2,...,r_n\right)}{kT}\right].$$

The calculation of these integrals at the present time can be easily carried out so far only for gases in which the particle density is small. A direct determination of the correlation functions of the melt with the help of statistical mechanics is quite difficult to perform. In such cases, one resorts to numerical methods, such as the Monte Carlo method, using the capabilities of computer technology. Suppose that we are interested in the mean value of some extensive physical property of the melt $M_n\left(r_1,r_2,...,r_n\right)$, determined by the mutual arrangement of a group of n-particles. In different areas of the melt, the configurations will differ from each other, so that the property values M_n will oscillate around this mean. Since the probability of the arrangement of particles in the configuration dW_n is described by the correlation function $F_n\left(r_1,r_2,...,r_n\right)$, the averaging of the quantity is performed by integrating M_n with the weight F_n:

$$\bar{M}_n=\int M_n\left(r_1,r_2,...,r_n\right)dW_n=\frac{1}{V^n}\int M_n\left(r_1,r_2,...,r_n\right)F_n\left(r_1,r_2,...,r_n\right)dV_1dV_2...dV_n=1.$$

In a melt containing N particles, the number of different groups of n-particles is equal $\frac{N!}{\left(N-n\right)!n!}$.

Therefore, the value of the property M_n for the entire volume of the melt will be:

$$M_n\left(N\right)=\frac{1}{V^n}\frac{N!}{\left(N-n\right)!n!}\int M_n\left(r_1,r_2,...,r_n\right)F_n\left(r_1,r_2,...,r_n\right)dV_1dV_2...dV_n.$$

Most often, properties are considered that depend either on the coordinate of one particle or on the mutual distances of pairs of particles, that is, properties determined by pair interactions. In the first case:

$$\bar{M}_1\left(N\right)=\frac{N}{V}\int M_1\left(r_1\right)F_1\left(r_1\right)dV_1.$$

It follows from equation (6) that $F_1\left(r_1\right)=\frac{V}{N}$, $R_1=\frac{V}{N}$, $R_0=1$, therefore:

$$\bar{M}_1\left(N\right)=\frac{N}{V}\int M_1\left(r\right)\,dV.$$

For a property defined by pair interactions, we can write:

$$\bar{M}_2\left(N\right)=\frac{N\left(N-1\right)}{2V^2}\int M_2\left(r_1,r_2\right)F_2\left(r_1,r_2\right)dV_1dV_2.$$

After some transformations we have:

$$\bar{M}_2\left(N\right)=\frac{R_0}{2}\int M_2\left(r_1,r_2\right)R\left(\left|r_2-r_1\right|\right)dV_1dV_2.$$

Denoting $\left|r_2-r_1\right|$ by r, we write:

$$\bar{M}_2\left(N\right)=2\pi N\int_0^\infty M_2\left(r\right)R\left(r\right)r^2dr. \qquad (7)$$

An important example of the application of equation (7) is the computation of the total energy of the melt in the approximation, when the potential energy of the system can be represented as the sum of the energies of the pair interaction of the particles. If the pair potential is denoted by $U\left(r\right)$ and take into account that the average kinetic energy of a monatomic particle is equal to $\frac{3}{2}kT$, then the following relationship holds for the total energy:

$$U=\frac{3}{2}NkT+2\pi N\int_0^\infty U\left(r\right)R\left(r\right)r^2dr.$$

The results described above show that knowledge of correlation functions $F_1, F_2, ..., F_n$ is necessary for the calculation of a number of thermodynamic properties of the melt. It will be shown below that the kinetic properties of melts in a number of cases are expressed in terms of integrals containing different correlation functions [4-10]. Therefore, it is expedient to set the problem of calculating correlation functions of lower orders through known potentials of interatomic interaction $U(r)$.

This problem was solved by a number of scientists: M. Born, G. Green, J. Kirkwood, N.N. Bogolyubov and others. As a result, rather complicated integro-differential equations connecting the functions F_n and F_{n+1}

$$F_1(r_1) = \frac{V}{N} R_1(r_1) = \frac{V}{N} R_0 = 1;$$

$$F_2(r_1, r_2) = \frac{V^2}{N(N-1)} R_2(r_1, r_2) \approx \frac{V^2}{N^2} R_2(r_1, r_2);$$

$$F_3(r_1, r_2, r_3) = \frac{V^3}{N(N-1)(N-2)} R_3(r_1, r_2, r_3) \approx \frac{V^3}{N^3} R_2(r_1, r_2, r^3).$$

Now the Bogolyubov-Born-Green equation for the index takes the form:

$$kT \nabla_1 R_2(r_1, r_2) + R_2(r_1, r_2) \nabla U(|r_1 - r_2|) + \int \nabla_1 U(|r_1 - r_3|) R_3(r_1, r_2, r_3) dV_3 = 0.$$

Here we took into account what is the interaction energy of two particles, that is. Dividing this equation by a function $R_2(r_1, r_2)$, we obtain the equation in the form proposed by M. Born and G. Green:

$$-kT \nabla_1 R_2(r_1, r_2) = \nabla U(|r_1 - r_2|) + \int \nabla_1 U(|r_1 - r_3|) \frac{R_3(r_1, r_2, r_3)}{R_2(r_1, r_2)} dV_3. \tag{8}$$

The equations obtained are rather complicated and a general method for their solution is not yet available. Successful results were obtained only for the simplest problems: for a system with low density (i.e., for a real gas), for a system of particles interacting according to the Coulomb law and for some other cases. A sufficiently exact solution can be obtained if a function F_S can be expressed in terms of functions F_n with smaller numbers $(n - S)$. Then it would be possible to «break off» the infinite system of equations (8) and find correlation functions, for example, by the method of successive approximations [5, 6]. One of the methods of approximate integration of the Bogolyubov-Born-Green equations was proposed by J. Kirkwood [7]. Taking into account the superposition approximation [7], the Bogolyubov-Born-Green equation (8) takes the form:

$$kT \ln R\;(r) + U(r) + \frac{2\pi N}{rV} \int_0^\infty [R(\rho) - 1] \left\{ \int E(x) x dx \right\} \rho d\rho = 0.$$

The solutions of this Bogolyubov-Born-Green equation for various particular cases were obtained by the method of successive approximations with the help of electronic computers. A new method for analyzing equations for correlation functions was proposed [7]. Without dwelling on it in essence, we note that the Percus-Yevick method [8] leads to the following integro-differential equation for the radial distribution function:

$$\exp[U(r)/kT] \cdot R\;(r) = 1 - \frac{N}{V} \int_0^\infty \left[\exp\left[\frac{U(r)}{kT}\right] - 1 \right] R(r') [U(|r - r'|)] dV'$$

which is the basis for calculating the radial distribution function of atoms in the melt.

The resulting equation describes the state of the melt and can describe its dynamics from a microscopic point of view. In this case, the potential energy of the particles depends on pair potentials of the type

$$U(r_1, r_2, ..., r_N) = \sum_{i<k}^{N} U(|r_i - r_k|).$$

Then, using the results of [8], we can write the expressions for the shear viscosity and of bulk viscosity:

$$\mu_{sh} = \rho_0 k_B T \left[1 + \frac{4}{15} I_1 + \frac{1}{15} I_2 \right] \tau;$$

$$\mu_V = \rho_0 k_B T \left[\frac{3}{5} - \frac{2}{9} I_1 + \frac{1}{9} I_2 \right] \tau - k_0 \tau,$$

where the integrals I_1, I_2, which depend on the paired potential $U(r)$ and the radial distribution function $R(r)$:

$$I_1 = \frac{2\pi\rho_0}{k_B T}\int_0^\infty R(r) r^3 \nabla_r U(r) dr;$$

$$I_2 = \frac{2\pi\rho_0}{k_B T}\int_0^\infty R(r) r^4 \nabla_r^2 U(r) dr.$$

Then, using known functions $U(r)$, $R(r)$ it is possible to calculate all the necessary values of the shear and bulk viscosities that appear in the equations of hydrodynamics.

Based on the analysis of the existing methods of building potential functions of inter-particle interaction in melts be obtained design formulae of atoms radial distribution functions in the system with the aim of obtaining basic data for building models of inter-particle interaction.

The mathematical models and methods developed in the work offer the approach to the solution of a fundamental problem of a method of molecular dynamics to the adequate description of potential of inter-particle interaction used in molten systems.

Besides, to analyze influence of the mechanism of inter-particle interaction in melts and the system properties that gives the chance to penetrate more deeply into the nature of the molten systems and to use this data in developing new technologies for metallurgical repartitions.

References

1 Seifert U. Stochastic thermodynamics: principles and perspectives / U. Seifert // Eur. Phys. J. — 2008. — Vol. 64B. Nos. 3–4. — P. 423–431.

2 Регель А. Физические свойства электронных расплавов / А.Р. Регель, В.М. Глазов. — М.: Наука, 1980. — 296 с.

3 Demchenko P.F. Applying modern methods of statistical physics to describe fluctuations of soil moisture reserve / P.F. Demchenko, L.D. Krasnokutskaya // Water Resources. — 2013, March. — Vol. 40. — Issue 2. — P. 133–142.

4 Kazhikenova S.Sh. On an algorithm for calculating the correlation functions for metallic melts /S.Sh. Kazhikenova // Scientific horizons – 2015. Materials of the XI International scientific and practical conference. September 30 – October 7, 2015. — UK, 2015. — Vol. 11. — P. 6–11.

5 Shimizu A. A numerical analysis of vortex growth in a two-dimensional jet / A. Shimizu, T. Wada // Comput. and Fluids. — 1985. — 13. — № 1. — P. 83–97.

6 Samarskii A.A. Computer simulation in engineering hydrodynamics / A.A. Samarskii, B.P. Gerasimov, T.G. Elizarova, I.S. Kalachinskaya, A.V. Karagichev, A.V. Lesunovsky, S.A. Semushin, B.I. Chetverushkin, A.G. Churbanov // Int. Symp. Comput. Fluid Dyn. — Tokyo, 1985. — P. 1007–1010.

7 Fischer I. Relationship between free energy density functional Born-Green-Yvon and potential distribution apparatus for in trowogeneus fluids / I. Fischer, V. Heinbush // J. Chem. Phys. — 1988. — 88. — № 3. — P. 1909–1913.

8 Suda M. New pair potentials from an improved Born-Green integral equation. Application to liquid metals / M. Suda // J. Phys. — 1983. — B50. — № 1. — P. 1–7.

9 Eshghinejadfard A. Numerical simulation of heat transfer in particulate flows using a thermal immersed boundary lattice Boltzmann method / A. Eshghinejadfard, D. Thévenin // International Journal of Heat and Fluid Flow. — 2016. — Vol. 60. — P. 31–46.

10 A. Xu. A three-dimensional pseudo-potential-based lattice Boltzmann model for multiphase flows with large density ratio and variable surface tension / A. Xu, T.S. Zhao, L. An, L. Shi // International Journal of Heat and Fluid Flow. — 2015. — Vol. 56. — P. 261–271.

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Корреляциялық функцияларды анықтау үшін рекурренттік қатынастар

Ішкі үйкелісін басудан туындаған балқыма бөлшектердің қозғалысы мен олардың өзара іс-қимылын басу күшінің тұтқыр қозғалыс металдық балқыманың математикалық сипаттамасының негізгі мәселелері қарастырылған. Зерттеудің жаңалығы корреляциялық функцияның тұтқырлығы кванттық статистикалық әдісі тұрғысынан қарастырылғандығында болып табылады. Корреляциялық функциялар мен радиалды функцияларды бөлу арасындағы өзара байланыс орнатылды. Сонымен қатар балқыма ағымының кластерлік теориясы негізінде тұтқырлық пен атомаралық потенциал арасында да байланыс орнатылды. Табылған қатынастар кез келген физикалық параметрлердің орташа мәнін анықтауға мүмкіндік берді. Дербес жағдайда ығысу мен көлемдік тұтқырлықты, сондайақ потенциалдық энергия жүйесі бөлшектердің өзара қозғалыс байланысының жұптық энергиясының қосындысы түрінде берілді. Физикалық параметрлердің орташа мәнін анықтау үшін екі бөлшекті функцияларды радиалды бөлу жеткілікті. Дербес жағдайда балқытылған металдардың коэффициенттерін ауыстыру болып табылады. Үш немесе одан да көп ретті корреляциялық функцияларды есептеу рекуррентті формулалары арқылы жүргізілді.

Кілт сөздер: металдық балқыту, гидродинамика теңдеулері, корреляциялық функциялар, кванттық потенциалдар, кванттық-статистикалық, математикалық модельдеу, компьютерлік модельдеу, тығыздық функционалы.

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Рекуррентные соотношения для определения корреляционных функций

Рассмотрена основная проблема математического описания вязкого движения металлического расплава, сопровождающегося преодолением внутреннего трения, обусловленного движением частиц расплава и преодолением сил их взаимодействия. Новизна исследований заключается в том, что корреляционные функции вязкости обоснованы с точки зрения квантово-статистического метода. Установлена взаимосвязь корреляционных функций с функциями радиального распределения. На основании кластерной теории течения расплава установлена связь между вязкостью и межатомным потенциалом. Найденные соотношения позволяют определить средние значения любых физических параметров, в частности значения сдвиговой и объемной вязкостей, а также представить потенциальную энергию системы в виде суммы энергий парного взаимодействия частиц. Двухчастичные функции радиального распределения достаточны для определения средних значений физических параметров, в частности коэффициентов переноса расплавленных металлов. Учет трех и более порядков корреляционных функций можно произвести по рекуррентным формулам.

Ключевые слова: металлический расплав, уравнения гидродинамики, корреляционные функции, квантовые потенциалы, квантово-статистический, математическое моделирование, компьютерное моделирование, функционал плотности.

References

1 Seifert, U. (2008). Stochastic Thermodynamics: Principles and Perspectives. *Eur. Phys. J.,* Vol. 64B, nos. 3–4, 423–431.

2 Regel, A.R., & Glazov, V.M. (1980). *Fizicheskie svoistva elektronnykh rasplavov [Physical properties of electron melts]*. Moscow: Nauka [in Russian].

3 Demchenko, P.F., & Krasnokutskaya L.D. (2013). Applying modern methods of statistical physics to describe fluctuations of soil moisture reserve. *Water Resources, March, Vol. 40,* Issue 2, 133–142.

4 Kazhikenova, S.Sh. (2015). On an algorithm for calculating the correlation functions for metallic melts. Scientific horizons – 2015. *Materials of the XI International scientific and practical conference.* September 30 – October 7, 2015. UK. (Vol. 11, pp. 6–11).

5 Shimizu, A., & Wada, T. (1985). A numerical analysis of vortex growth in a two-dimensional jet. *Comput. and Fluids, 13,* 1, 83–97.

6 Samarskii, A.A., Gerasimov, B.P., Elizarova, T.G., Kalachinskaya, I.S., Karagichev, A.V., Lesunovsky, A.V., Semushin, S.A., Chetverushkin, B.I., & Churbanov. A.G. (1985). Computer simulation in engineering hydrodynamics. *Int. Symp. Comput. Fluid Dyn,* 1007–1010. Tokyo.

7 Fischer, I., & Heinbush, V. (1988). Relationship between free energy density functional Born-Green-Yvon and potential distribution apparatus for in trowogeneus fluids. *J. Chem. Phys., 88,* 3, 1909–1913.

8 Suda, M. (1983). New pair potentials from an improved Born-Green integral equation. Application to liquid metals. *J. Phys., B50,* 1, 1–7.

9 Eshghinejadfard, A., & Thévenin, D. (2016). Numerical simulation of heat transfer in particulate flows using a thermal immersed boundary lattice Boltzmann method. *International Journal of Heat and Fluid Flow, Vol. 60,* 31–46.

10 Xu, A., Zhao, T.S., An, L., & Shi, L. (2015). A three-dimensional pseudo-potential-based lattice Boltzmann model for multiphase flows with large density ratio and variable surface tension. *International Journal of Heat and Fluid Flow, Vol. 56,* 261–271.