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SELF-CONSISTENT CALCULATIONS OF THE DYNAMIC, THERMODYNAMIC AND ELASTIC PRO-PERTIES OF A LATTICE OF ATOMIC CRYSTALS

The application of the self-consistent phonon theory (SCPT) formulated by Plakida and Siklós on the basis of the double-time Green's function method to the atomic crystals: rare gas solids (RGS), quantum crystals (QC) and metallic crystals (MC) is discussed. The special attention is given in theoretical investigation of the dynamic, thermodynamic and elastic properties of fcc and bcc structures using the reduced all-neighbours approximation of SCPT. The interatomic interactions in the mentioned crystals are described by the various models, among them by the generalized (exp,m) Buckingham, (n,m) Lennard-Jones and (exp,exp) Morse self-consistent potentials. The potential parameters are determined self-consistently with the help of the zero-point experimental data: the lattice constant, sublimation energy, compressibility and Debye characteristic temperature. Within numerical calculations we study the influence of the number of "important" shells of neighbours on temperature and pressure variations of the selected physical properties of atomic crystals. The computed results are compared with available experimental data.

Keywords: self-consistent phonon theory, properties of atomic crystals.

1. INTRODUCTION

The theory of lattice dynamics founded on the classical work by Born and Kàrmàn in its most simple approximation, in the harmonic approximation, is considered to be a well established theory capable to describe many of the

physical properties of the crystals in terms of independent normal models-phonons [1]. For a more precise description the anharmonicity of lattice vibrations or the interaction between the phonons should be taken into account and usually the ordinary perturbation theory considering the cubic and quartic interaction is quite appropriate for this purpose [2]. However, the investigations [3] showed that this approach cannot be applied in certain cases: near the phase transition points, e.g. melting point; for the quantum crystals with large zero-point energy; for the light impurities with small binding energy, etc., when the anharmonic effects are not small. Thus, many modifications of the theory of lattice dynamics of highly anharmonic crystals was elaborated simultaneously and independently by several authors by a variety of techniques. In one of these is the self-consistent phonon theory (SCPT) based on the variational principle [4,5]. A selective resummation of diagrammatic perturbation theory was used in [6]. The SCPT based on the thermodynamic double-time Green's function was proposed by Plakida and Siklós [7]. Today this version of SCPT is considered to be well established theory and it can be applied for investigation of dynamic, thermodynamic and elastic properties in a wide range of temperature and external pressure.

In the present paper the special attention is given to theoretical investigations of the physical properties of fcc and bcc lattices of RGS, QC and MC using the reduced all-neighbours approximation of the self-consistent phonon theory (RANASCPT).

The lattice atoms of simple atomic crystals with spherical symmetry interact with mainly central forces [8]. The long-range attractive interactions are of van der Waals-London (vdW-L) type and the short-range repulsion is connected with the quantum-mechanical effect of the overlapping of outer electronic shells of interacting atoms. Detailed theoretical consideration lead to the power (r^{-6}) and the exponential laws, respectively, for the attraction and repulsion portion of the pairwise atomic interaction in such crystals [9]. Earlier results of theoretical calculations allows us to state that among the functions for the initial pair interactions in atomic crystals the most common form was the (12,6) Lennard-Jones potential with parameters obtained usually from fits to experimental crystalline state properties [10].

It should be noted that the repulsion term (r^{-12}) appearing in the above mentioned function is not well founded theoretically from quantum mechanics [9] and thus a more realistic repulsive potential was desired. Singh and Neb [11] have constructed a model consist of the attractive vdW-L force modified by the variable induced dipoles and the repulsive Born-Mayer interactions.

Relative merits of Singh and Neb potential curve have been tested in our papers [12,13] by calculating the dynamic, thermodynamic [12] and elastic [13]

properties of strongly anharmonic heavier RGS by the help of nearest-neighbours approximation of the reduced second-order self-consistent phonon theory (NNARSOSCPT). The results of papers [12,13] compared with the principal theoretical data given in [14] for the Morse, Rydberg and Varshni self-consistent (s.c.) potentials showed that the best results as compared with experimental data were obtained for the purely exponential (*exp,exp*) Morse s.c. potential. Next, we have tested the applicability of the Morse potential together with the purely power generalized form of the (*n,m*) Lennard-Jones and mixed power-exponential (*exp,m*) Buckingham potentials to the description of the pressure variations of the limiting temperatures of dynamical and thermodynamical stability, selected thermodynamic functions and elastic properties of heavier RGS [15].

More recently [16,17], the above three s.c. models of pairwise interactions have been used for calculations of the most characteristic properties of solid He-3 and He-4 with the help of NNARSOSCPT [16] and RANASCPT [17].

It should be noted that the traditional (*12,6*) Lennard-Jones as well as its generalized (*n,m*) form were used in [10,18,19] for calculations of the dynamic and thermodynamic properties of metallic crystal with the help of the SCPT.

The all-neighbours approximation together with the five-parameters generalized Morse potential, with parameters obtained by Akgün and Uğur [20], and the classical (*exp,exp*) Morse s.c. potential was applied, last time, for investigations of the dynamic, thermodynamic [21,22] and elastic [23] properties of fcc metallic crystals, particularly properties of Ni fcc lattice.

In the present work a review of theoretical studies of dynamic, thermodynamic and elastic properties of atomic crystals in the RANASCPT is given. The main results obtained with the help of generalized form of the (*exp,m*) Buckingham, (*n,m*) Lennard-Jones and (*exp,exp*) Morse renormalized potentials for the lattices of heavier rare gas solids and quantum crystals are shown. In the case of metallic crystals interatomic interaction are represented in this paper by two versions of the Morse pair potential: classical, which is the four parameter one and modified by Akgün and Uğur [20] which is the five parameter.

2. RENORMALIZED POTENTIALS OF CRYSTALS IN THE REDUCED ALL-NEIGHBOUR APPROXIMATION OF THE SCPT

Using the general formula derived by Plakid and Siklós [7] for the s.c. potential we get the following analytical expression for the Buckingham $\tilde{\Phi}_b(l)$,

Lennard-Jones $\tilde{\Phi}_{LJ}(l)$, classical Morse $\tilde{\Phi}_M(l)$ [17] and the modified by Akgün and Uğur Morse $\tilde{\Phi}_{M^*}(l)$ renormalized potentials [22]:

$$\tilde{\Phi}_B(l) = C_B \left[\frac{1}{\alpha} x_1 \exp(\alpha y) - \sum_{k=0}^{\infty} \frac{1}{k!} y^k A_m^{(2k)} x_2^{m+2k} \right] \quad (1)$$

$$\tilde{\Phi}_{LJ}(l) = C_{LJ} \sum_{k=0}^{\infty} \frac{1}{k!} y^k [A_n^{(2k)} x_2^{n+2k} - A_m^{(2k)} x_2^{m+2k}] \quad (2)$$

$$\tilde{\Phi}_M(l) = C_M \left[\frac{1}{\alpha} x_1 \exp(\alpha y) - \frac{1}{\beta} x_3 \exp(\beta y) \right] \quad (3)$$

$$\tilde{\Phi}_{M^*}(l) = C_M x_2^\gamma \sum_{k=0}^{\infty} \left[\frac{1}{k!} y^k r_0^{2k} \sum_{j=0}^{2k} x_2^j (R_{kj} x_4 - A_{kj} x_5) \right], \quad (4)$$

The symbols used in (1)-(4) have the following meaning:

$$C_B = \frac{\alpha m D_0}{\alpha - m}, \quad C_{LJ} = \frac{nm D_0}{n - m}, \quad C_M = \frac{\alpha \beta D_0}{\alpha - \beta},$$

$$x_1 = \exp[\alpha(1 - l/r_0)], \quad x_2 = r_0/l, \quad x_3 = \exp[\beta(1 - l/r_0)],$$

$$x_4 = \exp(-\alpha/x_2), \quad x_5 = \exp(-\beta/x_2)$$

$$A_{p'}^{(q)} = \begin{cases} \frac{1}{p'} & \text{for } q=0 \\ \frac{1}{p'} p'(p'+1) \dots (p'+k-1) & \text{for } q=1,2,\dots \end{cases}$$

R_{kj} and A_{kj} are the matrixes defined in [22]. In equations (1)-(4) n , m , α and β are the dimensionless parameters describing the slope of the potential curves, r_0 and D_0 define the potential minimum and are, respectively, the equilibrium distance of two isolated atoms and the energy of their dissociation. The equation (4) for $y = 0$ is equivalent to the original of Akgün and Uğur one [20] and was obtained by the following substitutions:

$$r_0 = r_0^{AU}, \quad D_0 = D_0^{AU}, \quad \gamma = n^{AU}, \quad \beta = \alpha^{AU} r_0^{AU}, \quad \alpha = m^{AU} \alpha^{AU} r_0^{AU}$$

Factor x_2 should exhibit the correct nature of the interatomic forces in metallic crystals, particularly at short distance [22].

The renormalization parameter y appearing in Eqs. (1)-(4) is equal to:

$$y = \frac{\langle u^2(l) \rangle}{2r_0^2} \quad (5)$$

where: $\langle u^2(l) \rangle = \langle [\bar{l}(\bar{u}_i - \bar{u}_0)]^2 \rangle / l^2$. \bar{u}_0 and \bar{u}_i are the displacements of neighbouring atoms from their equilibrium positions and \bar{l} is their equilibrium separation. $\langle u^2 \rangle$ depends on the explicit form of s.c. pairwise atomic interaction $\tilde{\Phi}(l)$ and the temperature range. In particular, for the strongly anharmonic crystals under an arbitrary external pressure p and temperature T we get [7]:

$$\langle u^2(T, p) \rangle \approx 6\theta C_0(T, p) \left[\left(1 - 0.11 \frac{\beta(T, p)}{\theta} \right)^{-1} + C_3(T, p) \right] \quad (6)$$

The exact expression for the symbols using in (6) are given in [22].

The relations (1) to (6) form the system of s.c. equations which determines the potential energy of pairwise interactions of atoms at fixed temperature and pressure. Of course, the potential energy of crystal consists of energies of interaction of all pair of atoms. However, in order to describe the above quantity and all other physical properties of crystal lattice we should, at first, calculate all unknown parameters appearing in each of Eqs (1) to (4). These parameters are fitted to experimental data of zero-point internal energy U_0 , zero-point volume V_0 , zero-point bulk modulus B_T and the Debye characteristic temperature θ_D determine at low temperatures using the modified Fürth [24] and Shu Zen and Davies [10] method. These modification [17] allows us to determine the parameters of s.c. potentials functions as they depend on the number of shells “ i ” of nearest neighbours z_i having an influence on the pair interactions. Obtained analytical set of equation for the $\tilde{\Phi}_B(l)$, $\tilde{\Phi}_L(l)$, $\tilde{\Phi}_M(l)$ potential parameters is given in [17] and in [22] for $\tilde{\Phi}_{M^*}(l)$ and were used as the first approximation in our numerical calculations of parameters for the four mentioned model renormalized potentials.

Having the values of potential constants for the pairwise atomic interaction in considered crystals we can calculate the pressure and temperature variations of y (Eqs (5) and (6)) and the anharmonic force constants $f(T, p)$ and $g(T, p)$ defined, respectively, as the second and third derivatives of the s.c. potential $\tilde{\Phi}(l)$. Then all dynamic and thermodynamic properties of strongly anharmonic crystals may be expressed as functions of y , $\tilde{\Phi}(l)$, $\tilde{\Phi}''(l)$ and $\tilde{\Phi}'''(l)$ but the respective equations must take into account the potential energy of crystals obtained in the higher approximation with respect to the number of acting neighbours.

3. GENERAL EQUATION OF STATE, THERMODYNAMIC FUNCTIONS AND THE ISOTHERMAL ELASTIC CONSTANTS IN THE RANASCPT

In the nearest-neighbouring (n.n.) approximation of the SCPT the simplifying assumption was taken by Plakida, Siklós and Aksienov [7,25,26] that each atom interacts only with its n.n. In this paper we try to reject this assumption incorporating further shells “*i*” and the number of atoms z_i in such *i*-th shells in the s.c. equations. Then, the equation of state takes the following form [17]:

$$p(z_i) = p \left[1 + \sum_{i=2}^{i_{\max}} \frac{l_i}{l} \frac{z_i}{z} \frac{\tilde{\Phi}'(l_i)}{\tilde{\Phi}'(l)} \right] \quad (7)$$

In the same way, the internal energy per atom $E(z_i)$ and enthalpy $H(z_i)$ are equal to:

$$E(z_i) \approx E + \sum_{i=2}^{i_{\max}} \frac{1}{2} z_i \tilde{\Phi}(l_i), \quad H(z_i) \approx E(z_i) + p(z_i)V \quad (8,9)$$

where p , l , z , E and V denote, respectively, the equation of state, distance between neighbouring atoms, number of n.n., internal energy and the specific volume in the n.n. approximation [26]. According to the thermodynamic relations [27] the difference between the molar heats at constant pressure and constant volume is equal to:

$$C_p(z_i) - C_v(z_i) = T \left(\frac{\partial p(z_i)}{\partial T} \right)_V \left(\frac{\partial V}{\partial T} \right)_p$$

and

$$T [C_p(z_i) - C_v(z_i)] = \left[p(z_i) + \left(\frac{\partial E(z_i)}{\partial V} \right)_T \right] \cdot \left[V - \left(\frac{\partial H(z_i)}{\partial p(z_i)} \right)_T \right]. \quad (10)$$

This formula express a general thermal equation of state for crystal characterized by the molar heats and thermodynamic functions – the internal energy and enthalpy in the reduced, all neighbours approximation of the self-consistent phonon theory.

The temperature and pressure variations of the isothermal elastic constant $c_{\alpha\beta}(T,p)$ of considered atomic crystals can be obtained with the help of the following formula [7]:

$$c_{\alpha\beta}(T,p) = c_{\alpha\beta}^h \alpha_1(T,p) [1 - 2\beta_1(T,p) S_{ij}] \gamma(T,p), \quad (11)$$

where

$$\alpha_1(T,p) = \frac{f(T,p)}{f}, \quad \beta_1(T,p) = \frac{k_B T g^2(T,p)}{f^3(T,p)}, \quad \gamma(T,p) = \frac{l}{l(T,p)}$$

The quantities $c_{\alpha\beta}^h$, f , k_B and $S_{\vec{k}_j}$ are, respectively, the harmonic elastic constant, harmonic second-order force constant, Boltzmann constant and the coefficient defined by the direction of the wave vector \vec{k} and polarization \vec{j} yielding the corresponding elastic constants c_{11} , c_{44} and $c_{11}-c_{12}$ [7].

Using the above modified s.c. equations (Eqs. (7)-(11)) we can test the relative merits of the four forms (Eqs. (1)-(4)) renormalized potentials by calculating the temperature and pressure dependent properties of the fcc and bcc lattices of atomic crystals. As it was mentioned in section 2 of this paper in the respective equations we must take into account the fact that the potential energy of crystal consist of energies of interactions of all pair of atoms.

4. NUMERICAL RESULTS

Using as starting point an analytical results for the potential parameters given in our previous papers [17,22] we were fitting by trial-and-error method the four s.c. potentials for considered crystals (RGS, QC, MC) to the lowest-pressure experiment trying to predict the experimental values of the lattice constant, compressibility and the internal energy with the help of RANASCPT. The respective calculations were being carried out for various i_{max} of shells of neighbours – up to 10 and over – and the results, as an example, are presented in Table 1 for the He-4. The number of shells taken into account is limited to 10 as it appeared that the values of parameters obtained for $i_{max}= 10$ and for instance 20 are generally nearly the same, while those for $i_{max}= 1$ and for 10 differ very distinctly.

Table 1
Optimal values of the Buckingham (B), Lennard-Jones (LJ) and Morse (M) s.c. pair potentials parameters for He-4 vs. the number of shells of neighbours [17]

Potential	i_{max}	n	m	α	β	r_0 (10^{-10} m)	D_0 (10^{-21} J)
(B)	1	-	6.0	4.5	-	2.91290	0.098666
	5	-	6.0	4.5	-	3.07372	0.101246
	10	-	6.0	4.5	-	3.07214	0.104952
(LJ)	1	10.2	5.1	-	-	2.86295	0.105345
	5	10.2	5.1	-	-	2.98160	0.076050
	10	10.2	5.1	-	-	3.00550	0.071710
(M)	1	-	-	6.0	3.0	2.69110	0.093480
	5	-	-	6.0	3.0	3.52450	0.042310
	10	-	-	6.0	3.0	3.82740	0.034900

Optimal values of the parameters of various models of interatomic interactions in rare gas solids (RGS), quantum crystals (QC) and metallic crystals (MC) calculated in the highest approximation with respect to the number of shells of neighbours are collected in Table 2.

Table 2
Optimal values of the Buckingham, Lennard-Jones and Morse pair potential parameters for the heavier RGS, QC and MC

Potential parameters	Ar			Kr			Xe		
	$(\alpha,6)B$	$(n,6)LJ$	$(\alpha,\beta)M$	$(\alpha,6)B$	$(n,6)LJ$	$(\alpha,\beta)M$	$(\alpha,6)B$	$(n,6)LJ$	$(\alpha,\beta)M$
n or α [-]	14.26	12.28	13.50	14.92	12.96	13.20	13.91	11.81	13.00
β [-]	-	-	5.36	-	-	5.86	-	-	5.46
r_0 [10^{-10} m]	3.7909	3.7952	3.7756	4.0532	4.0586	4.0299	4.4279	4.4378	4.4041
D_0 [10^{-21} J]	1.7485	1.6995	1.9977	2.4393	2.3791	2.8512	3.3726	3.2603	3.8902
	He-3			He-4			Ni		
	$(\alpha,m)B$	$(n,m)LJ$	$(\alpha,m)M$	$(\alpha,m)B$	$(n,m)LJ$	$(\alpha,m)M$	$(\alpha,\beta)M$	$(\alpha,\beta)M^*$ ($\gamma = 0.44$)	
n [-]	-	7.2	-	-	10.2	-	-	-	
m [-]	6	3.6	-	6	5.1	-	-	-	
α [-]	3	-	6	4.5	-	6	10.53	10.53	
β [-]	-	-	3	-	-	3	5.24	4.66	
r_0 [10^{-10} m]	3.40930	3.30300	3.07214	3.00550	3.82740	3.68158	2.549	2.576	
D_0 [10^{-21} J]	0.05979	0.03558	0.10495	0.07171	0.03490	0.04846	45.6	44.47	

As a test of validity of both the models of interatomic interactions (respectively Buckingham, Lennard-Jones, classical and modified Morse potentials with parameters given in Table 1 and 2) and the model of lattice dynamics (the reduced all-neighbours approximation of the SCPT) we have computed the equilibrium distance between neighbouring atoms l , the internal energy E (Table 3 and 4) and the isothermal bulk modulus B_T (Table 5) for the heavier RGS (Ar, Kr and Xe), QC (He-3 and He-4) and MC (Ni). Theoretical results are collected as an example, for two values of temperature ($T = 0K$ and $T = T_m$ – the melting temperature) and in the case of QC for a few values of high pressure. We are paying a special attention to l , E and B_T because just for these quantities exist experimental data and we can show their comparison with theoretical results.

Table 3

The nearest neighbours separation l and the internal energy E as function of pair potential and temperature for RGS and MC. Experimental values [30-32] for $T = T_m$ are given for comparison

Potential		$l [10^{-10} \text{ m}]$			$-E [10^{-21} \text{ J/atom}]$		
		$(\alpha,6)B$	$(n,6)LJ$	$(\alpha,\beta)M$	$(\alpha,6)B$	$(n,6)LJ$	$(\alpha,\beta)M$
Ar	$T = 0\text{K}$	3.7480	3.7480	3.7480	12.8202	12.8199	12.8201
	$T = T_m$	3.9016	3.9241	3.8842	9.8423	9.6554	9.9832
	experiment	3.857			-		
Kr	$T = 0\text{K}$	3.9920	3.9919	3.9920	18.5350	18.5349	18.5350
	$T = T_m$	4.1739	4.1954	4.1460	13.7105	13.4435	13.9865
	experiment	4.125			-		
Xe	$T = 0\text{K}$	4.3350	4.3350	4.3350	26.6210	26.6212	26.6213
	$T = T_m$	4.5377	4.5646	4.5152	19.5803	19.2626	19.8496
	experiment	4.492			-		
Potential		$(\alpha,\beta)M^*$		$(\alpha,\beta)M$	$(\alpha,\beta)M^*$		$(\alpha,\beta)M$
Ni	$T = 0\text{K}$	2.4784		2.4759	-331.21		-332.14
	$T = T_m$	2.5806		2.5599	-254.330		-263.61
	experiment	2.478 for $T = 0\text{K}$			-331.20 for $T = 0\text{K}$		

Table 4

Pressure variations of the nearest neighbours separation l and internal energy E in QC as a function of pair potential at $T = 0\text{K}$. Experimental values [28,29] are given for comparison. $i_{max} = 20$

Potential	He-3				He-4			
	$p \text{ (MPa)}$				$p \text{ (MPa)}$			
	3.516	5.218	7.691	10.051	3.222	6.414	9.646	14.256
$l [10^{-10} \text{ m}]$								
$(\alpha,m)B$	3.7270	3.6516	3.5679	3.5055	3.6378	3.5514	3.4863	3.4157
$(n,m)LJ$	3.7270	3.6465	3.5586	3.4936	3.6378	3.5480	3.4819	3.4112
$(\alpha,\beta)M$	3.7270	3.5906	3.4562	3.3634	3.6378	3.4609	3.3464	3.2318
experiment	3.7270	3.6477	3.5648	3.5073	3.6378	3.5468	3.4835	3.4178
$E [10^{-24} \text{ J / atom}]$								
$(\alpha,m)B$	-14.5	5.4	32.1	55.9	-79.8	-53.2	-28.8	3.5
$(n,m)LJ$	-14.5	8.5	39.2	66.3	-79.8	-59.5	-37.6	-6.6
$(\alpha,\beta)M$	-14.5	-4.7	10.5	25.3	-79.8	-59.8	-39.0	-9.7
experiment	-14.5	-3.9	11.9	26.6	-79.8	-68.0	-54.9	-35.3

Table 5

The isothermal bulk modulus B_T as function of pair potential and temperature for RGS, QC and MC. Experimental values [30-32] for $T = T_m$ are given for comparison

		B_T [Gpa]		
Potential		$(\alpha,6)B$	$(n,6)LJ$	$(\alpha,\beta)M$
Ar	$T = 0K$	2.6699	2.6705	2.6680
	$T = T_m$	0.7779	0.6269	0.9301
	experiment	1.14		
Kr	$T = 0K$	3.4510	3.4510	3.4515
	$T = T_m$	0.8917	0.7338	1.1576
	experiment	1.33		
Xe	$T = 0K$	3.5816	3.5791	3.5792
	$T = T_m$	1.0005	0.8193	1.2017
	experiment	1.38		
Potential		$(\alpha,m)B$	$(n,m)LJ$	$(\alpha,\beta)M$
He-3	$T = 0K$ $p = 3.516MPa$	0.0103	0.0828	0.01259
He-4	$T = 0K$ $p = 3.222MPa$	0.0068	0.0080	0.01633
Potential		$(\alpha,\beta)M^*$		$(\alpha,\beta)M$
Ni	$T = 0K$	182.001		182.690
	$T = T_m$	89.306		88.309
	experiment	182.0 for $T = 0K$		

5. CONCLUSION

The main results of this paper are the following:

- Analytical results for quantities describing dynamic, thermodynamic and elastic properties of fcc and bcc lattices of atomic crystals as they depend on the number of “important” shells “ i ” of nearest neighbours z_i are given.
- The calculations in the reduced all-neighbours approximations of the self-consistent phonon theory (based on the double-time Green’s function method) are presented. Interatomic potential functions are described by the generalized (exp,m) Buckingham, (n,m) Lennard-Jones, classical (exp,exp) Morse and the modified by Akgün and Uğur (for metallic crystals) Morse self-consistent potential.
- Selected numerical results are shown for heavier rare gas solids, quantum crystals and metallic crystals. The computed results for the equilibrium distance between neighbouring atoms l , internal energy E and the isothermal bulk modulus B_T are compared with available measured data.

Bearing in the mind this comparison as well as the results of our earlier papers [15,17,22] we hope that all self-consistent potentials considered here represented quite-good the real interatomic forces in strongly anharmonic crystals of light and heavier RGS. Analytical results given in this paper can be used for description of the dynamics and thermodynamics of other class of atomic crystals with spherical symmetry.

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WŁAŚCIWOŚCI DYNAMICZNE, TERMODYNAMICZNE I SPRĘŻYSTE KRYSZTAŁÓW PIERWIASTKÓW W TEORII POLA SAMOUZGODNIONEGO

Streszczenie

W pracy przedstawiono wyniki badań właściwości dynamicznych, termodynamicznych i sprężystych kryształów pierwiastków gazów szlachetnych (RGS) oraz kryształów kwantowych (QC) i metalicznych (MC). Analityczny opis został wykonany w przybliżeniu wszystkich sąsiadów teorii pola samouzgodnionego Plakidy i Siklósa, opartej na metodzie dwuczasowych temperaturowych funkcji Greena. Oddziaływania międzyatomowe w sieci ww. kryształów pierwiastków aproksymowano uogólnionymi 4-parametrowymi krzywymi (exp, m) Buckinghama, (exp, exp) Morse oraz (n, m) Lennarda-Jonesa. Parametry krzywych potencjalnych zostały wyznaczone w funkcji liczby powłok „ i ” kolejnych sąsiadów (tab. 1 i 2) w oparciu o dane doświadczalne dla stałych sieci, energii sublimacji, ściśliwości oraz temperatury charakterystycznej Debye’a. Szczegółowe obliczenia numeryczne dla odległości najbliższych sąsiadów l , energii wewnętrznej E (tab. 3 i 4) oraz izotermicznego modułu sprężystości B_T (tab. 5) dla trzech grup kryształów pierwiastków zostały porównane z danymi doświadczalnymi.