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REALISTIC INTERATOMIC POTENTIAL FOR MD SIMULATIONS

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The coefficients of interatomic potential of simple form Exp-6 for neon are obtained. Repulsive part is calculated ab-initio in the Hartree-Fock approximation using the basis of atomic orbitals orthogonalized exactly on different lattice sites. Attractive part is determined empirically using single fitting parameter. The potential obtained describes well the equation of state and elastic moduli of neon crystal in a wide range of interatomic distances and it is appropriate for molecular dynamic simulations of high- temperature properties and phenomena in crystals and liquids.

1. Introduction

Investigation of strongly anharmonic nonlinear atomic systems by molecular dynamics (MD) method at high temperatures, pressures, or study of systems affected by large amplitude excitations requires high accuracy of interatomic potential (IP). Series expansion of the IP in the displacements of atoms from equilibrium positions is widely used both in phonon theory and in MD simulation [1,2]. Usually, fourth-order anharmonisms or lower-order ones can be taken into account because of complexity of expansion coefficients calculation. As an alternative, realistic potential method is used [3–5], in which exact equations of motion of atoms are solved using IP of a concrete substance without series expansion. Owing to that, all-order anharmonisms are taken into account automatically. This advantage of realistic potential method is especially useful in the MD simulation of soliton solutions where atoms approach each other closely. Realistic IP should have the simplest form to reduce calculation expenses as well as it must describe precisely the properties of the substance under extreme conditions. The aim of this paper is to obtain such IP.

Conventional way of realistic IP determination is the empirical fitting to the properties of a gas or a crystal near the equilibrium point [6,7]. However, such potentials become unreliable at small interatomic distances like that arising in soliton waves. The properties of highly compressed matter (e.g., for neon up to 1Mbar [8]) could give an information for obtaining all-distance reliable IP. However, the set of properties, which can be measured accurately at megabar pressures, is restricted strongly. Practically, only the equation of state and bulk modulus may be included in this set [8,9]. For shear elastic moduli C_{ik} the precision worsens drastically even at kilobar pressures [10,11]. The empirical information for fitting all the parameters of IP is insufficient, and *ab-initio* calculation is required.

Realistic IP via interatomic distance is obtained in the present work for the crystal and dimer of neon. The repulsive part of the potential is calculated *ab-initio* in the Hartree-Fock approximation using the basis of localized atomic orbitals orthogonalized exactly on different lattice sites. The attractive part is chosen to have the standard Van-der-Vaals form of Cr^{-6} with single empirical parameter C. The used approximations and calculation details are described in section 2. In section 3, the repulsive part of IP is interpolated by exponential function of interatomic distance (Exp-6 potential) and the IP parameters are determined. Experimental verification of the IP obtained is performed in section 4 using the data concerning equation of state [8,9] and elastic moduli [12–17] of compressed neon. The IP calculated is found to be in a good consistency with the experiment in the whole of pressure range.

2. *Ab-initio* calculation of repulsion potential

In MD simulations by realistic potential method the problem is divided into two stages. The former is quantum-mechanical calculation of the IP at electron level, with interatomic distance considered as a parameter. The latter is solving the equations of motion of atoms using the IP obtained. This division corresponds to adiabatic approximation when motion of atoms and electrons is described separately [18].

Since pair collisions of atoms have maximal probability, we concentrate the attention on the dimer of neon, and define the IP as a cohesive energy of the dimer. Three-atom forces can be taken into account as a correction to the two-atom ones using incremental expansion [19]. The estimation of [19] shows three-atom force contribution to be small.

In Hartree-Fock approximation, the short-range repulsive part of IP is expressed through one–electron density matrix. We don’t use hard core approximation. Rearrangement of all electron shells is allowed as the interatomic distance is altered.

Localized basis of atomic orbitals orthogonalized exactly (by Lovdin procedure [20]) on different lattice sites is used. In this basis, one-electron density matrix has the form [21]:

$$\rho(\mathbf{r}'|\mathbf{r},\{\mathbf{l}\}) = 2\sum_{\mathbf{l}s}\left\{\varphi_s(\mathbf{r}'-\mathbf{l})\varphi_s^*(\mathbf{r}-\mathbf{l}) - \sum_{\mathbf{l}'s'}\varphi_{s'}(\mathbf{r}'-\mathbf{l}')P_{s's}^{\mathbf{l}'\mathbf{l}}\varphi_s^*(\mathbf{r}-\mathbf{l})\right\} \qquad (1)$$

$$\mathbf{P} = \mathbf{I} - (\mathbf{I}+\mathbf{S})^{-1},$$

where $\varphi_s(\mathbf{r}-\mathbf{l}) = |\mathbf{l}s\rangle$ is the wave function of electron in isolated atom (atomic orbital), $\mathbf{l}$ and $\mathbf{l}'$ are radius-vectors of lattice sites, s numerates the occupied states of the atom, $\mathbf{P}$ is the orthogonalizing matrix, $\mathbf{I}$ is the unit matrix, $\mathbf{S}$ is the overlap integral matrix with the elements

$$S^{\mathbf{l}'\mathbf{l}}_{s's} = \langle \mathbf{l}'s'|\mathbf{l}s\rangle \text{ when } \mathbf{l}\neq\mathbf{l}'; \quad S^{\mathbf{l}'\mathbf{l}}_{s's} = 0 \text{ when } \mathbf{l}=\mathbf{l}'. \qquad (2)$$

We expand the repulsive part of IP in terms of small parameter such as the largest overlap integral S. Usually, $S << 1$ in uncompressed crystal, and overlap integrals grow exponentially as interatomic distance is decreased. The IP is expressed through the products of elements of orthogonalizing matrix **P** and two-center Slater-Koster integrals. These integrals are atomic obital matrix elements of crystal hamiltoinian operators. The order in S for two-center integrals is estimated using the mean-value theorem. The elements of matrix $\mathbf{P} = \mathbf{I} - (\mathbf{I} + \mathbf{S})^{-1}$ are expanded in powers of the overlap integral matrix **S**

$$P^{\mathbf{ll}'}_{ss'} = S^{\mathbf{ll}'}_{ss'} + O(\mathbf{S}^2),\ P^{\mathbf{ll}}_{ss'} = -(\mathbf{S}^2)^{\mathbf{ll}}_{ss'} + O(\mathbf{S}^3), \qquad (3)$$

where s numerates the occupied states of the atom, **S** is the complete matrix of overlap integrals. The elements of matrix **P** contain high-order terms along with the main ones proportional to S and S^2.

Using the estimations described above, we expand the repulsive part of IP in powers of S

$$V_{sr} = E^{(0)} + W_2 + W_4 + W_6. \qquad (4)$$

Here $E^{(0)}$ is the energy of interatomic interaction if orthogonalization of neighboring atoms orbitals is neglected, W_2, W_4, W_6 are orthogonalizing corrections. Series expansion in S begins for them from the second, the third, and the sixth powers respectively. Due to the presence of matrix **P,** the orthogonalizing corrections contain high-order terms in S along with the main ones.

In equation (4)

$$E^{(0)} = \sum_{\mathbf{l}s}\ \sum_{\mathbf{m},\mathbf{m}\neq\mathbf{l}} \left\langle \mathbf{l}s \middle| V^{\mathbf{m}}_{en} + V^{\mathbf{m}}_{a} + V^{\mathbf{m}}_{ex} \middle| \mathbf{l}s \right\rangle + U_{nn}. \qquad (5)$$

The first term in equation (5) consists of two-center integrals. They are the atomic orbital matrix elements of electron-ion interaction potential $V^{\mathbf{m}}_{en}$, of neutral isolated atom potential $V^{\mathbf{m}}_{a}$, of electron-electron exchange interaction potential $V^{\mathbf{m}}_{ex}$, respectively. The second term is the energy of nucleus-nucleus interaction. The electron-ion interaction potential has the form

$$V^{\mathbf{m}}_{en} = V_{en}(\mathbf{r}-\mathbf{m}) = -Ze^2/\left|\mathbf{r}-\mathbf{m}\right|. \qquad (6)$$

Neutral isolated atom potential is

$$V^{\mathbf{m}}_{a} = V_a(\mathbf{r}-\mathbf{m}) = V_{en}(\mathbf{r}-\mathbf{m}) + 2\sum_t \left\langle \mathbf{m}t \middle| v_c \middle| \mathbf{m}t \right\rangle, \qquad (7)$$

where

$$\left\langle \mathbf{m}t \middle| v_c \middle| \mathbf{m}t \right\rangle = \int \varphi^*_l(\mathbf{r}'-\mathbf{m})\, v_c(\mathbf{r}-\mathbf{r}')\, \varphi_t(\mathbf{r}'-\mathbf{m})\, \mathrm{d}\mathbf{r}'; \quad v_c(\mathbf{r}-\mathbf{r}') = e^2/|\mathbf{r}-\mathbf{r}'|.$$

Action of electron-electron exchange interaction potential on wave function is defined as

$$\left\langle \mathbf{l}s\left|V_{ex}^{\mathbf{m}}\right|\mathbf{l}s\right\rangle = -\sum_{t}\left\langle \mathbf{l}s\,\mathbf{m}t\right|v_c\left|\mathbf{l}s\,\mathbf{m}t\right\rangle . \tag{8}$$

In equation (4), the orthogonalizing corrections, W_2, W_4, W_6, are of the form

$$W_2 = -2\sum_{\mathbf{l}s}\;\sum_{\mathbf{l}'s',\mathbf{l}\neq\mathbf{l}'} P_{ss'}^{\mathbf{l}\mathbf{l}'}\left\langle \mathbf{l}'s'\left|V_a^{\mathbf{l}'}+V_{ex}^{\mathbf{l}'}\right|\mathbf{l}s\right\rangle -$$

$$-\sum_{\mathbf{l}\mathbf{m}ss'tt',\,\mathbf{l}\neq\mathbf{m}} P_{ss'}^{\mathbf{m}\mathbf{l}}\,P_{tt'}^{\mathbf{l}\mathbf{m}}\left\langle \mathbf{l}s'\,\mathbf{m}t'\right|v_c\left|\mathbf{m}s\,\mathbf{l}t\right\rangle ; \tag{9}$$

$$W_4 = \sum_{\mathbf{l}\,ss'tt'} P_{ss'}^{\mathbf{l}\mathbf{l}}\,P_{tt'}^{\mathbf{l}\mathbf{l}}\left\{2\left\langle \mathbf{l}s'\,\mathbf{l}t'\right|v_c\left|\mathbf{l}t\,\mathbf{l}s\right\rangle - \left\langle \mathbf{l}s'\,\mathbf{l}t'\right|v_c\left|\mathbf{l}s\,\mathbf{l}t\right\rangle\right\} -$$

$$-2\sum_{\mathbf{l}\,ss'} P_{ss'}^{\mathbf{l}\mathbf{l}}\left\langle \mathbf{l}s'\left|\sum_{\mathbf{m}\neq\mathbf{l}} V_a^{\mathbf{m}}+V_{ex}^{\mathbf{m}}\right|\mathbf{l}s\right\rangle +$$

$$+2\sum_{\mathbf{l}\mathbf{m}ss'tt',\mathbf{l}\neq\mathbf{m}}\left\{P_{ss'}^{\mathbf{l}\mathbf{l}}\,P_{tt'}^{\mathbf{m}\mathbf{m}}\left\langle \mathbf{l}s'\,\mathbf{m}t'\right|v_c\left|\mathbf{m}t\,\mathbf{l}s\right\rangle + P_{ss'}^{\mathbf{m}\mathbf{l}}\,P_{tt'}^{\mathbf{l}\mathbf{m}}\left\langle \mathbf{l}s'\,\mathbf{m}t'\right|v_c\left|\mathbf{l}t\,\mathbf{m}s\right\rangle\right\} +$$

$$+\sum_{\mathbf{l}\mathbf{m}ss'tt',\,\mathbf{l}\neq\mathbf{m}} P_{ss'}^{\mathbf{m}\mathbf{l}}\,P_{tt'}^{\mathbf{m}\mathbf{l}}\left\{2\left\langle \mathbf{l}s'\,\mathbf{l}t'\right|v_c\left|\mathbf{m}t\,\mathbf{m}s\right\rangle - \left\langle \mathbf{l}s'\,\mathbf{l}t'\right|v_c\left|\mathbf{m}s\,\mathbf{m}t\right\rangle\right\} +$$

$$+4\sum_{\mathbf{l}\mathbf{m}ss'tt',\mathbf{l}\neq\mathbf{m}} P_{ss'}^{\mathbf{m}\mathbf{l}}\,P_{tt'}^{\mathbf{l}\mathbf{l}}\left\{2\left\langle \mathbf{l}s'\,\mathbf{l}t'\right|v_c\left|\mathbf{l}t\,\mathbf{m}s\right\rangle - \left\langle \mathbf{l}s'\,\mathbf{l}t'\right|v_c\left|\mathbf{m}s\,\mathbf{l}t\right\rangle\right\}; \tag{10}$$

$$W_6 = -\sum_{\mathbf{l}\mathbf{m}ss'tt',\mathbf{l}\neq\mathbf{m}} P_{ss'}^{\mathbf{l}\mathbf{l}}\,P_{tt'}^{\mathbf{m}\mathbf{m}}\left\langle \mathbf{l}s'\,\mathbf{m}t'\right|v_c\left|\mathbf{l}s\,\mathbf{m}t\right\rangle . \tag{11}$$

Since the orthogonalizing corrections grow exponentially as the interatomic distance is decreased, it is impossible to say which correction may be neglected. It should be checked for each substance under consideration.

Using the method described, we calculate the repulsive part of IP, V_{sr} (equation (4)), for neon dimer as a function of interatomic distance d. Atomic orbitals from Clementi-Roetti set [22] are used as a basis. Hartree system of atomic units $\hbar = e = m_e = 1$ is applied. The calculation shows the terms $E^{(0)}$ and W_2 in equation (4) to have the same order of magnitude and opposite signs. These terms are found to give major contributions to the IP. The W_4 correction consists of 0.02% of the IP at equilibrium interatomic distance d_0. Further, the W_4 does not exceed 1% of the IP up to $d \sim 0.75d_0$. Finally, at small d, like that arising in soliton waves (for d above 0,6–$0.75d_0$), the W_4 becomes about 2–4% of the IP. The contribution of W_6 to the IP is negligible (~0.002%) in the whole range of d under consideration.

3. Determination of interatomic potential parameters

We interpolate the calculated points $V_{sr}(d)$ by exponential function of interatomic distance, using the least square method, by the formula

$$V_{sr}(d) = A_0 \exp(-\alpha(x-1)), \quad x = d/z_0 \qquad (12)$$

with two unknown parameters A_0 and α. Experimental equilibrium interatomic distance for neon dimer z_0 = 5.8411 a. u. [23] is used as the third parameter of the IP. The parameters are found to be A_0 = $(1,1384 \mp 0,0002)\cdot 10^{-4}$ a. u., α = = 13.6407 ∓ 0.0037. Interpolation error is 1–4% of V_{sr} when the d is altered from $0.6z_0$ to equilibrium one.

Adding the attractive part, we express the IP in standard Exp-6 form

$$V(d) = A_0 \exp(-a(x-1)) - \tilde{N}d^{-6}, \quad x = d/z_0 \, . \qquad (13)$$

A single unknown parameter C remains in the attractive part of IP. We propose to fit the C to experimental equilibrium interatomic distance. The using of equilibrium data is considered to be reliable at all interatomic distances since the attraction is essential near the equilibrium only, while *ab-initio* calculated repulsive part dominates at small d.

For MD simulation of lattice dynamics, it is possible to fit the C to experimental data for dimer at $T = 0$ because the temperature effects will be taken into account explicitly, at the stage of solving the equations of motion. In this case, for neon C = 10.7293 (experimental equilibrium interatomic distance in the dimer is z_0 = 5.8411 a. u. [23]). The calculated cohesive energy of dimer is $E_{\text{coh}} = -1.4497\cdot 10^{-4}$ a. u., the experimental one is $E_{\text{coh}} = -1.338\cdot 10^{-4}$ a. u. [23]. The discrepancy is 7% of the experimental value.

For calculating static properties of a crystal at finite temperature, e.g. the equation of state, elastic moduli, it is better to fit the C to experimental data for a crystal at the same temperature. Such determination allows to take into account implicitly the three-atom forces, temperature effects, zero-point oscillations, and other effects omitted at the stage of IP calculation. In this case, for neon C = 7.4030 (experimental equilibrium interatomic distance in the crystal is d_0 = 5.9647 a. u. at T = 4.25 K [12]). The calculated cohesive energy of incompressed crystal is $E_{\text{coh}} = -6.7620\cdot 10^{-4}$ a. u. per atom, the experimental one is $E_{\text{coh}} = -(7.35 \pm 0.03)\cdot 10^{-4}$ a. u. [24]. The discrepancy is 7.6% of the experimental value.

4. Results and discussion

Interatomic potential of neon is given in Fig. 1 as a function of interatomic distance d.

The IP calculated by equation (13) for dimer is plotted by solid curve. Van-der-Vaals constant (C = 10.7293) is fitted to experimental equilibrium interatomic distance in dimer [23].

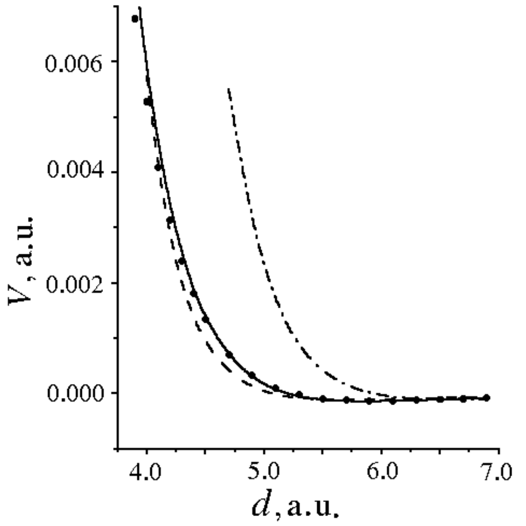


Fig. 1. Calculated IP and potentials fitted to experimental data for neon. Exp-6 is the potential interpolated by formula (13), 6–12 is the potential interpolated by (14). ● – Exp-6, crystal, 1 Mbar [8]; ——— – Exp-6, dimer, calculation; - - - - - 6–12, compressed gas [6]; -·-·- – 6–12, crystal, $p = 0$

«Experimental» IP obtained in [8] is denoted by solid circles. This IP has been determined by interpolating the experimental data $p(V)$ (measured at 300 K) by the formula Exp-6. The interpolation has been performed in theoretical model taking thermal pressure and zero-point oscillations into account explicitly, excluding them from the definition of IP. It allows us to compare the 300 K data of [8] with zero-temperature result of this paper. Three-atom forces were not included explicitly in the model of [8]. However, in [8], the effect of these forces is taken into account implicitly through fitting the IP to experimental data for the crystal. In our calculation, three-atom forces are omitted because of fitting to dimer data. The agreement of calculated IP and experimental one indicates that three-atom forces in neon are small at pressures up to 1Mbar.

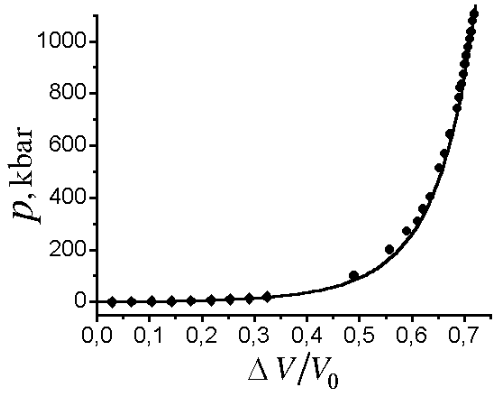
Dashed and dashed-dotted curves in the figure 1 are interatomic potentials of neon obtained by fitting to experimental data using the Lennard-Jones potential (6–12 formula)

$$V(x) = \varepsilon\,(-2/x^6 + 1/x^{12}),\quad x = d/z_0, \tag{14}$$

where ε and z_0 are fitting parameters. Dashed curve is the IP obtained using the low of corresponding-states fitted to vapor-pressure ratio of isotopic liquid [6]. Dashed-dotted curve is the IP fitted to experimental lattice constant and cohesive energy of crystal neon at $p = 0$, $T = 0$ [7]. Fitting to equilibrium crystal properties leads to a bad describing the IP for compressed crystal. Fitting to compressed gas properties gives the values of the IP close to experimental ones at moderate pressures.

Using the IP obtained (13) we calculate the equation of state $p(V)$ for solid neon. Calculated pressure p against fractional volume is given in Fig. 2 as solid curve.

Van-der-Vaals constant is fitted to experimental equilibrium interatomic distance $d_0 = 5.9647$ a. u. measured for crystal neon at $T = 4.25$ K, $p = 0$ [12].



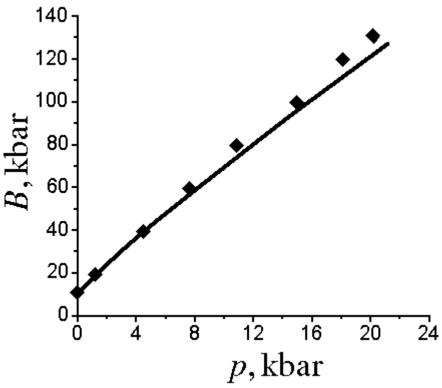


Fig. 2. Plot of $\Delta V/V_0$ as a function of p for solid neon. ◆ – experiment, $T = 4.2$ K [9]; ● – experiment, $T = 300$ K [8]; —— – calculation, $T = 0$ K

Fig. 3. Bulk elastic modulus of solid neon. —— – calculation, $T = 0$, ◆ – experiment, $T = 4.2$ K [9]

Experimental points $p(V)$ from [8] (T = 300 K) and [9] (T = 4.2 K) are also given in Fig. 2. At the pressures below 20 kbar the theoretical curve is in a good agreement with the experimental points of [9]. At moderate pressures the theoretical curve deviates from experimental points of [8] by 4%. This deviation is caused, mainly, by neglecting the thermal pressure in our calculation. Fig. 2 shows temperature sensitivity of the equation of state to be small.

We calculate bulk modulus of solid neon by means of the IP obtained. Van-der-Vaals constant is fitted to experimental equilibrium interatomic distance in the crystal [12]. Calculated bulk modulus B via the pressure p is given in Fig. 3 as solid curve.

Experimental points obtained in [9] at T = 4.2 K are plotted as solid symbols. Bulk modulus is seen to be more sensitive to the approximations used. Growing when the p is enhanced, the difference between calculated B and measured one becomes about 7% of experimental B at p = 20 kbar. Incorrect taking three-atom forces into account at moderate pressures seems to contribute mainly to this discrepancy. In our calculation, three-atom forces (and zero-point oscillations too) are taken into account implicitly, by fitting the IP to experimental data for uncompressed crystal. Thus, calculated B agrees with experimental one at low pressures only (to 8 kbar). One can't determine correctly the dynamics of alteration of three-atom forces with the enhancement of pressure. This is the cause of growing the deviation of calculated B from measured one.

We calculate elastic moduli C_{ik} using the IP obtained with Van-der-Waals constant fitted to crystal experimental data [12]. Calculated moduli and experimental ones are given in table for uncompressed solid neon at low temperatures. Isothermic moduli have been obtained in static measurements [9,12]. Adiabatic moduli have been measured in ultrasonic and neutron scattering experiments [13–17]. However, the difference between isothermic moduli and adiabatic ones is negligible at the temperatures under consideration (see, e.g., [13]).

Table

Elastic moduli of solid neon

Ref.	T, K	B, kbar	C_{11}, kbar	C_{12}, kbar	C_{44}, kbar	$d = (C_{44} - C_{12})/C_{12}$	Method
[12]	4.25	11.12±0.12	–	–	–	–	Static. measurements of $p(V)$
[9]	4.2	11.0±0.1	–	–	–	–	
[13]	4	11.36±0.26	–	–	–	–	Ultrasonic velocity measurements
[14]	5	11.2±0.5	–	–	–	–	
[15]	4.7	12.1±0.4	16.9±0.5	9.7±0.4	10.0±0.3	0.03±0.07	Inelastic neutron-phonon scattering
[16]	5	11.24±0.17	16.61±0.17	8.55±0.21	9.52±0.05	0.11±0.03	
[17]	6	11.52±0.3	16.49±0.3	9.03±0.3	9.28±0.08	0.03±0.04	
Calc	0	10.76	14.95	8.67	8.67	0	*Ab-initio* calc.

The C_{ik} moduli are seen to be more sensitive to the measurement method and calculation approximations. The difference between theoretical and experimental values of C_{11} and C_{44} is about 10% of experimental values for the most accurate experiment [16]. The agreement is better for C_{12} modulus (the discrepancy is about 2% [16]). The deviation from Cauchy relation $\delta = (C_{44} - C_{12})/C_{12}$ is also given in the table. Cauchy violation is the measure of deviation of the IP from spherical symmetry. The $\delta = 0.11 \pm 0.03$ in [19], while it falls into experimental error bar in other experiments listed in the table. Cauchy relation takes place for our calculation results because in theoretical model the IP is supposed to be of spherical symmetry form. Small value of experimental δ indicates that spherical symmetry approximation for IP is valid for uncompressed neon at least. For another rare gas crystal, krypton, experiment [11] shows Cauchy relation to satisfy well under pressure up to 80 kbar. Moreover, for MgO the Cauchy violation is measured to drop with enhancing pressure up to 200 kbar [25].

Unlike C_{ik} moduli, bulk modulus B is less sensitive to measurement method and calculation approximations. The discrepancy of theoretical result and experimental one doesn't exceed 4% and falls into experimental error frames.

5. Conclusion

Coefficients of realistic IP of simple form Exp-6 are obtained for neon by *ab-initio* calculation of the repulsive part in Hartree-Fock approximation in the basis of atomic orbitals orthogonalized exactly on different lattice sites. The attractive part is determined empirically using the single fitting parameter, Van-der-Vaals constant *C*. For fitting the *C* it is enough to know experimental equilibrium interatomic distance in crystal (or dimer), i.e. high-pressure experimental data is not required. The IP calculated is suitable for molecular dynamic simulations of high-temperature and high-pressure properties and phenomena in crystals and liquids due to simplicity of the form and precise describing experimental data in wide range of interatomic distances.

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