Dispersion of acoustic excitations in tetrahedral liquids

Yu D Fomin

Vereshchagin Institute of High Pressure Physics, Russian Academy of Sciences, 108840 Kaluzhskoe shosse, 14, Troitsk, Moscow, Russia
Moscow Institute of Physics and Technology, 9 Institutskiy Lane, Dolgoprudny City, Moscow Region, Russia

Received 18 December 2019, revised 15 May 2020
Accepted for publication 22 May 2020
Published 23 June 2020

Abstract
Investigation of the longitudinal and transverse excitations in liquids is of great importance for understanding the fundamentals of the liquid state of matter. One of the important questions is the temperature and density dependence of the frequency of the excitations. In our recent works it was shown that while in simple liquids the frequency of longitudinal excitations increases when the temperature is increased isochorically, in water the frequency can anomalously decrease with the temperature increase. In the present manuscript we study the dispersion curves of longitudinal and transverse excitations of water and liquid silicon modelled by Stillinger–Weber (SW) potential. We show that both in liquid silicon and SW model of water the frequencies of longitudinal excitations slightly increase with temperature which is in contrast to the results for SPC/E model of water.

Keywords: collective excitations in liquids, dispersion curves, anomalies of liquids, tetrahedral liquids, molecular simulation
(Some figures may appear in colour only in the online journal)

1. Introduction
It is well known that some liquids (for instance, water, silicon, silica, carbon, phosphorus, etc) can demonstrate anomalous behavior in the vicinity of their freezing lines [1–16]. The most widespread example is water. Its phase diagram has regions where the slope of the melting line is negative (melting of ordinary ice), thermal expansion coefficient has negative value (density anomaly), diffusion coefficient increases under isothermal densification (diffusion anomaly), viscosity decreases when the density increases isothermally (viscosity anomaly), etc. Other liquids from the list of examples above also demonstrate some anomalous features. Moreover, one can see that these liquids are very different (water is a molecular liquid, silicon is a metallic liquid, silica is an ionic one, etc). Because of this it becomes of principle importance to find out some general mechanisms responsible for the appearance of anomalous properties in so different substances.

Several models were introduced in the literature to explain the appearance of the anomalous behavior in the liquids. For instance, Stell and Hemmer introduced a concept of potentials with negative curvature (or core-softened models) [17, 18]. The core-softened potentials are characterized by softening of the repulsive part of the interaction potential between the particles [19]. The concept of core-softened systems appeared to be very useful for investigation of complex phase diagrams and liquid state anomalies (see the review [20] and references therein). Many different core-softened models were proposed and studied by different groups of researchers. It was found that the behavior of the core-softened models is very sensitive to the details of the interaction potential. Because of this choosing an appropriate potential one can qualitatively reproduce some anomalous features of water or other liquids. Moreover, such models are simpler for studying. Therefore, one can use them as a simplified model to obtain some results, which can be after that found in real substances. An example of such approach, where the results obtained for a core-softened model were then discovered in a model of water is given in references [21, 22].

Another important class of liquids which demonstrate anomalous behavior is related to the tetrahedral liquids [23, 24]. First of all, water belongs to the tetrahedral liquids. Other examples of the tetrahedral liquids are silicon, germanium, tin and carbon. Importantly, some of these liquids demonstrate
anomalous behavior (water and silicon, carbon), while others do not [23, 24]. Let us discuss it in more details.

Basing on the results of computer simulation it was shown that liquid silicon demonstrate numerous anomalies similar to the ones of water [23, 26–28]. Density anomaly, structural anomaly, diffusion and viscosity anomaly were predicted in liquids silicon. Moreover, it was predicted that silicon experiences a liquid–liquid phase transition in supercooled region [26]. Similar predictions were made for water [29]. However, in the case of water it was predicted that the liquid–liquid critical point is located at the (P, T) parameters inaccessible for experiments (so called ‘no man’s land’). Because of this computer simulation became the main tool to study liquid–liquid phase transition in water.

Silicon has high melting temperature. Although it is possible to perform experiments with liquid silicon, it meets some difficulties: aside from the high melting point one should mention very low viscosity and extremely high chemical reactivity of liquid silicon. Because of this there is lack of experimental data on liquid silicon. On the other hand, computer simulations of liquid silicon are mostly based on classical empirical potentials. At the same time it is known, that crystalline silicon is semiconductor while liquid silicon is metal. Therefore, the electronic structure is dramatically change upon melting. The classical potentials used to simulate liquid silicon are constructed on the basis of the data for crystalline silicon (lattice constant, binding energy, etc) and therefore they should not be strictly valid for the liquid phase. Liquid silicon was also studied by ab initio computer simulations, which overcomes the limitations of the interaction potential mentioned above. However, ab initio methods suffer on other limitations (small systems, small simulated times, etc). From this discussion one can see that classical models of silicon have only limited applicability and can pretend on some qualitative description of liquid silicon only. However, because of the limitations of experimental and ab initio methods they are still of wide usage.

Stillinger and Weber proposed a model potential for silicon (SW potential) [30]. Later on this model was generalized to describe other tetrahedral liquids [23–25]. It is composed of two- and three-body terms. Importantly, the three-body term includes a parameter λ called the ‘tetrahedrality parameter’, since it controls the degree of tetrahedrality in the liquid: the higher value of lambda means more tetrahedral liquid (see the next section for more detailed description). Since some of the tetrahedral liquids demonstrate anomalous behavior while others do not, several studies were devoted to a comparison of their behavior in frames of the SW model [23, 24].

In reference [25] a parametrization of SW potential for water was proposed. The choice of the SW potential for simulation of water is supported by the tetrahedral nature of water. The authors used the following experimental data to fit the model: the melting point, the density of liquid and ice at the melting point, the enthalpy of melting and evaporation, the diffusion coefficient at T = 298 K, the liquid–vapor surface tension at T = 300 K and the density and temperature of the density anomaly at ambient pressure. From this list one can see that the model was fitted mostly to the properties close to the melting line. Because of this the SW model of water gives rather good results next to the melting line, but fails to reproduce experimental results at elevated temperature.

Reference [25] also reports a comparison of water with other tetrahedral liquids in the framework of SW model. According to this paper the largest tetrahedrality parameter corresponds to the case of carbon (λC = 26.2). In the case of water λH2O = 23.15. It becomes even smaller for silicon (λSi = 21.0) and germanium (λGe = 20). In the case of carbon the situation is very difficult due to extremely high melting temperature. Moreover, up to now there is no firm data for the melting temperature of graphite [31, 32]. Different publications give extremely different results. Even less is known about liquid carbon. One can expect numerous anomalies in liquid carbon, but neither experimental, nor theoretical methods give firm evidences. Water and silicon demonstrate anomalous properties, while germanium does not [23, 24]. Basing on this one can assume that anomalous behavior is expected for larger values of λ and becomes less pronounced and finally disappear as λ becomes smaller.

In reference [23] a study of the anomalous behavior of SW liquids with different tetrahedralities was performed. The authors added a model of tin with λSn = 18.5 in the set of liquids and investigated such anomalies as density anomaly, structural anomaly via pair entropy (see [33] for the discussion of different definitions of the structural anomaly), high values of isobaric heat capacity and anomaly of tetrahedral order parameter defined via a combination of angles between the particles within the first coordination shell. It was found that the anomalous properties are absent at large (carbon) and small (tin and germanium) values of λ, but they are present at some intermediate values (water and silicon). Therefore, the influence of tetrahedrality on the behavior of liquid appeared to be even more complex than it was supposed before.

A novel anomalous property was discovered in our previous works [21, 22]: anomalous dependence of frequency of longitudinal excitations in liquids at isochores: in a simple liquid the frequency of longitudinal excitations should increase with isochoric increasing of temperature, while in the anomalous liquids it can decrease. This anomaly was observer in computer simulation of SPC/E model of water and in a model core-softened system (repulsive shoulder system, RSS). The anomaly can also be found by investigation of the frequencies of longitudinal excitations along isotherms. However, in this case the anomaly is much less pronounced: the frequency shows extremely weak dependence on density in the anomalous region. This result is in qualitative agreement with experimental study reported in reference [34].

As we have seen from the discussion above, tetrahedral liquids can demonstrate anomalous behavior which strongly depends on the parameter of tetrahedrality. Basing on this fact, it is of great interest to monitor the behavior of anomaly of the dispersion of longitudinal excitations in liquids with different tetrahedrality. In the present paper we study the dispersion curves of water and liquid silicon—two the most anomalous tetrahedral liquids and show that in both cases the anomaly is absent, which is in contrast to the SPC/E model of water.
2. Systems and methods

In the present paper two systems are considered: liquid silicon and water, i.e. two tetrahedral liquids, which demonstrate anomalous behavior. Both of them are modeled by the SW potential. In the case of water it means that a molecule of water is considered as a single unified particle. The energy of a system with the SW potential is described by the following equation [30]:

\[ E = \sum_{i<j} \phi_2(r_{ij}) + \sum_i \sum_{j>i} \phi_3(r_{ij}, r_{ik}, \theta_{ijk}), \]  

where

\[ \phi_2(r_{ij}) = A_{ij} \varepsilon_{ij} \left( B_{ij} \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{n_0} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{n_1} \right) \exp \left( \frac{\sigma_{ij}}{r_{ij} - a_{ij}\sigma_{ij}} \right). \]  

\[ \phi_3(r_{ij}, r_{ik}, \theta_{ijk}) = \lambda_{ijk} \varepsilon_{ijk} \left( \cos \theta_{ijk} - \cos \theta_{ijk} \right)^2 \times \exp \left( \frac{\gamma_{ijk} \sigma_{ijk}}{r_{ij} - a_{ijk}\sigma_{ijk}} \right) \exp \left( \frac{\gamma_{ijk} \sigma_{ijk}}{r_{ik} - a_{ijk}\sigma_{ijk}} \right). \]  

The parameters of the potential for both silicon and water are given in Table 1. The difference in the potentials for silicon and water is in three parameters: depth of the potential well \( \varepsilon \), effective size of the particles \( \sigma \) and parameter of ‘tetrahedrality’ \( \lambda \): higher \( \lambda \) means higher tetrahedrality, i.e. water is more tetrahedral than silicon.

|        | Si         | Water      |
|--------|------------|------------|
| \( \varepsilon \) | 2.1683     | 0.268381   |
| \( \sigma \)  | 2.0951     | 2.3925     |
| \( a \)      | 1.80       | 1.80       |
| \( \lambda \) | 21.0       | 23.15      |
| \( \gamma \) | 1.80       | 1.20       |
| \( \cos(\theta_{ijk}) \) | -1/3       | -1/3       |
| \( A \)      | 7.05       | 7.05       |
| \( B \)      | 0.602      | 0.602      |
| \( p \)      | 4.0        | 4.0        |
| \( q \)      | 0.0        | 0.0        |

The simulation setup for water is similar to the one for liquid silicon. Time step is set to \( dt = 0.0005 \) ps. Equilibration period is 2 ns and the production period is 5 ns. Temperature varies from \( T_{\text{min}} = 1000 \) K to \( T_{\text{max}} = 2000 \) K. The temperature of minimum pressure is \( T_{\text{DA}} = 1300 \) K.

In the case of liquid silicon the system is equilibrated for 2 ns in canonical ensemble (constant number of particles \( N \), volume \( V \) and temperature \( T \)). After that long micro-canonical simulation (constant number of particles \( N \), volume \( V \) and internal energy \( E \)) for more 5 ns is performed. During this stage the properties of the system are calculated. The time step is \( dt = 0.0001 \) ps. The temperatures vary from \( T_{\text{min}} = 1300 \) K to \( T_{\text{max}} = 2000 \) K. The temperature of minimum pressure is \( T_{\text{DA}} = 1300 \) K.

In order to find the excitation frequencies the velocity current autocorrelation functions are calculated. The longitudinal and transverse parts of these functions are defined as:

\[ C_L(k, t) = \frac{k^2}{N} \langle J_x(k, t) \cdot J_x(-k, 0) \rangle \]  

and

\[ C_T(k, t) = \frac{k^2}{2N} \langle J_y(k, t) \cdot J_x(-k, 0) + J_z(k, t) \cdot J_y(-k, 0) \rangle \]  

where \( J(k, t) = \sum_{j=1}^{N} \mathbf{v}_j e^{-ikr_j(t)} \) is the velocity current and wave vector \( k \) is directed along the \( z \) axis [35, 36]. The dispersion curves of longitudinal and transverse excitations can be obtained as the location of maxima of Fourier transforms \( \tilde{C}_L(k, \omega) \) and \( \tilde{C}_T(k, \omega) \) respectively. All simulations were performed in lammps simulation package [39].

3. Results and discussion

3.1. Liquid silicon

In the present work we use a system with the SW potential is described by the following equation (1). The parameters for silicon are taken from reference [30] and the parameters for water from reference [25].

![Image](image.png)

Table 1. Coefficients SW potential for silicon and water equation (1). The parameters for silicon are taken from reference [30] and the parameters for water from reference [25].
Figure 1. (a) The equation of state of liquid silicon along the isochore $\rho = 2.503 \text{ g cm}^{-3}$. (b) The isochoric heat capacity of silicon at the same density.

Figure 2. (a) The radial distribution functions of liquid silicon along the isochore $\rho = 2.503 \text{ g cm}^{-3}$. (b) The structure factors of liquid silicon at the same density.

anomaly in the system, in agreement with previous works [23, 26–28]. Moreover, the isochoric heat capacity of liquid silicon has very high values at low temperature (figure 1(b)). Such behavior appears when liquid demonstrates a smooth structural crossover [37, 38]. This crossover can be seen from radial distribution functions (RDFs) and structure factors of the system shown in figure 2. Both RDFs and structure factors have complex shape. In the case of the RDFs the second peak has a shoulder at lower values of $r$, which means that the second coordination shell is scattered. This scattering should be responsible for the appearance of the density anomaly.

The complex nature of the local structure of liquid silicon is even more pronounced in structure factors (figure 2(b)). Structure factors demonstrate two clear peaks. At low temperatures the second peak appears to be higher than the first one. However, when the temperature increases the first peak goes up, while the second one goes down. Therefore, smooth change of the local structure is observed.

Basing on the presence of water-like anomalous behavior and smooth structural crossover the question is whether liquid silicon demonstrates anomalous dependence of the dispersion curves similar to the one observed in a model core-softened system [22] and SPC/E model of water [21, 22].

Figures 3(a) and (b) show the examples of Fourier image of longitudinal and transverse excitations of liquid silicon. Unlike the case of a simple liquid, these Fourier images cannot be approximated by a single peak, since they also demonstrate a shoulder at higher frequencies. This is consistent with the results for water obtained in references [40, 41]. In the present paper we consider the frequencies of the main peak only as it is the most powerful process in the system.
Figure 3. (a) Examples of Fourier image of longitudinal current autocorrelation functions of liquid silicon at $k = 0.592 \, \text{Å}$ at different temperatures. The left inset enlarges the region of maxima of the curves. The arrow indicates the direction of increasing of the temperature. The right inset enlarges the curve for $T = 1000 \, \text{K}$. (b) The same for the transverse excitations.

Figure 4. The dispersion curves of (a) longitudinal and (b) transverse excitations of liquid silicon at $\rho = 2.503 \, \text{g cm}^{-3}$ and different temperatures. The inset on the panel (a) gives a comparison of the dispersion curves at the lowest and highest temperatures studied ($T = 1000 \, \text{K}$ and $2000 \, \text{K}$). The inset on the panel (b) shows the width of the band-gap.

The location of maxima of the curves shown in figures 3 (a) and (b) follows normal regime: the frequency of the maximum increases with temperature for longitudinal excitations and decreases with a temperature increase for the transverse ones. However, the frequency shift of longitudinal excitations is extremely weak: while the temperature changes two-fold (from $T = 1000 \, \text{K}$ to $T = 2000 \, \text{K}$) the shift of frequency is just about 4%.

Figures 4(a) and (b) show the dispersion of longitudinal and transverse excitations of liquid silicon. One can see that longitudinal excitations demonstrate very modest temperature dependence. The inset of the panel (a) gives a comparison of the dispersion curves at the lowest and the highest temperatures ($T = 1000 \, \text{K}$ and $2000 \, \text{K}$ respectively). One can see that the difference between these curves does not exceed 4%. Although the changes in the frequency of the longitudinal excitations of liquid silicon are very modest, the frequency increases with temperature. Therefore, no anomaly is detected in this case.

Experimental measurements of the dispersion curve of liquid silicon at $T = 1733 \, \text{K}$ were reported in reference [42]. The experimental frequencies of longitudinal excitations are about twice less then the ones obtained in the present work for $T = 1700 \, \text{K}$. However, experiments and calculations of the present work were conducted at very different conditions: while experiments were performed under ambient pressure, the pressure in the current simulation at $T = 1700 \, \text{K}$ is $P_{\text{MD}} = 12.2 \, \text{kbar}$. Taking into account so dramatic difference in pressure, a direct comparison of the present calculations with experimental results is irrelevant.

The dispersion curves of transverse excitations behaves in an usual way: the frequency at some fixed wave vector $k$ decreases with temperature. At the lowest temperatures no band gap is observed. It appears at $T = 1700 \, \text{K}$. The width of the band gap increases with temperature. The width of the band gap becomes equal to the width of the first Brillouin zone.
Figure 5. (a) The equation of state of water along the isochore \( \rho = 0.997 \text{ g cm}^{-3} \). (b) The isochoric heat capacity of water at the same density.

at the Frenkel line [49–54]. From figure 4 it can be concluded that the temperatures of the present study are well below the Frenkel temperature of liquid silicon.

3.2. Water

The same analysis was performed for water. Figures 5(a) and (b) show the equation of state and the isochoric heat capacity of water along isochor \( \rho = 0.997 \). The equation of state demonstrates a minimum, i.e. the density anomaly. The isochoric heat capacity has very large value, i.e. smooth structural crossover takes place. This is very similar to the case of liquid silicon described above and to the behavior of the SPC/E water model [21, 22].

Figures 6(a) and (b) give the RDFs and structure factors of water. One can see that the structure of water changes rapidly on heating. While at low temperatures two clear peaks are observed, at high ones only the first peak with wide shoulder from right side is present. The same effect is seen in structure factors: two peaks at low temperatures and a single peak at high ones.

Figure 7(a) shows the dispersion curves of longitudinal excitations in water at \( \rho = 0.997 \) and a set of temperatures. One can see that at moderate wave vectors the temperature dependence of the frequency is like in a simple liquid, i.e. the frequency increases with temperature. The curves cross at \( k = 1 \text{ Å}^{-1} \), and the frequency at lower temperature becomes larger then the one at higher temperature. However, this value of \( k \) is out of the first Brillouin zone which is 0.75–0.8 Å\(^{-1} \) for different temperatures. Therefore, within the first Brillouin zone no anomalous dependence is detected. This is in contrast to the results for the SPC/E model of water [21, 22].

The transverse excitations of water behave as in a simple liquid, i.e. the frequency decreases with a temperature increase. Moreover, one can see unambiguous transverse excitations at the temperatures from \( T = 220 \text{ K} \) to \( T = 300 \text{ K} \). At
Figure 7. (a) The dispersion curves of longitudinal excitations of water at $\rho = 0.997 \text{ g cm}^{-3}$ and different temperatures. The inset on the panel (a) gives a comparison of the dispersion curves at the lowest and highest temperatures studied. (b) The dispersion curves of transverse excitations of water at the same density and the same set of temperatures. The notation of the curves of the panel (b) is the same that of the panel (a).

$T = 400 \text{ K}$ we do not observe well recognized transverse excitations. Therefore, the Frenkel temperature of the SW water is somewhere between 300 and 400 K.

One can see that the temperature dependence of the excitation frequencies of the SW model of water is qualitatively different from the one of the SPC/E model. In this respect it is necessary to find out which model gives more reliable results. The SPC/E model of water introduced in reference [43] is a three site model, i.e. a molecule of water is represented as oxygen atom bonded with two hydrogen ones. The SW model of water is a united model, i.e. the molecule of water is approximated by a single atom. The SW model is fitter to reproduce a number of properties of water in the vicinity of the melting line [25]. Although the excitation frequencies were not included in the fitting properties, SW model of water reproduces them quite well at $T = 300 \text{ K}$ and ambient pressure [41]. However, such a crude model cannot give precise results far from the region where it was fitted, which can be seen, for instance from the location of the Frenkel temperature which is between 300 and 400 K for the SW model of water, 460 K for the SPC/E model [44] and 520 K for the TIP4P/2005 model [45].

The SPC/E model also fails to reproduce the phase diagram of water [46, 47]. However, it gives reasonable estimate of the critical temperature [48]. Taking into account that in the present study we consider the high temperature properties of water, we believe that the spectra of the SPC/E model of water reported in references [21, 22] should be more trustworthy.

From the results above one can see that no liquid silicon, no water modeled by SW potential demonstrate anomalous behavior of the excitation spectra. Indeed, water and liquid silicon demonstrate many similar features, such as density anomaly, diffusion anomaly, viscosity anomaly, etc. In this respect similar behavior of the temperature behavior of the excitation spectra looks to be in line with other properties of these systems: in both cases the temperature dependence of the frequency is very weak, but the frequency always increases with temperature, i.e. no anomaly is found. However, it is in contrast to the results of more complex model of water, namely SPC/E one, which is discussed above. From this consideration, we can assume that tetrahedrality itself in not sufficient for the anomaly of the dispersion curves, and some molecular degrees of freedom which are taken into account in SPC/E model, are required.

4. Conclusions

In conclusion, we have examined the dispersion curves of both longitudinal and transverse excitations of liquid silicon and water in frames of SW potential models fitted for these substances. As it was shown before, the SPC/E model of water demonstrates anomalous temperature dependence of the frequency of longitudinal excitations: while in a simple liquid the frequency increases with temperature, in SPC/E model of water in can decrease. However, this effect was not observed in the SW model of water. In the case of liquid silicon we observe extremely weak temperature dependence of the longitudinal frequency, i.e. no anomaly is discovered. The behavior of transverse excitations is qualitatively similar in both liquid silicon and water: at fixed $k$-vector the frequency decreases with a temperature increase. At the same time the Frenkel temperature of liquid silicon appears to be very high (more then $T = 2000 \text{ K}$, which is the highest temperature of the present study), while in water the Frenkel temperature is somewhere between 300 and 400 K, i.e. very close to the melting point. Importantly, the SW models of both water and liquid silicon have numerous limitations, and because of this the results obtained within the framework of these models can be inconsistent with experiments. Because of this and taking into account the disagreement between the results for SW water and the SPC/E model of water we believe that novel experimental results are required to find out whether the anomaly of the dispersion curves exist in water or not.
Acknowledgments

This work was carried out using computing resources of the federal collective usage center ‘Complex for simulation and data processing for mega-science facilities’ at NRC ‘Kurchatov Institute’, http://ckp.nrcki.ru, and supercomputers at Joint Supercomputer Center of the Russian Academy of Sciences (JSCC RAS). The work was supported by the Russian Science Foundation (Grants No. 19-12-00111).

ORCID IDs

Yu D Fomin  
https://orcid.org/0000-0002-8344-4533

References

[1] Debenedetti P 2003 J. Phys.: Condens. Matter 15 R1669
[2] Buldyrev S V, Franzese G, Giovambattista N, Malescio G, Sadr-Lahiji M R, Scala A, Skibinsky A and Stanley H E 2002 Physica A 304 23
[3] Angell C A 2004 Annu. Rev. Phys. Chem. 55 559
[4] Debenedetti P G 1998 Metastable Liquids: Concepts and Principles (Princeton: Princeton University Press)
[5] V V Brazhkin, S V Buldyrev, V N Ryzhov and H E Stanley (ed) 2002 New kinds of phase transitions: transformations in disordered substances Proc. NATO Advanced Research Workshop Volga River (Dordrecht: Kluwer)
[6] Errington J R and Debenedetti P G 2001 Nature 409 318
[7] Netz P A, Starr F V, Stanley H E and Barbasoa M C 2001 J. Chem. Phys. 115 344
[8] Mishima O and Stanley H E 1998 Nature 396 329
[9] Angell C A, Finch E D and Bach P 1976 J. Chem. Phys. 65 3063
[10] Thurn H and Ruska J 1976 J. Non-Cryst. Solids 22 331
[11] Sauer G E and Borst L B 1967 Science 158 1567
[12] Prielmeier F X, Lang E W, Speedy R J and Lidemann H D 1987 Phys. Rev. Lett. 59 1128
[13] Prielmeier F X, Lang E W, Speedy R J and Lidemann H D 1998 Ber. Bunsenges. Phys. Chem. 92 1111
[14] Haar L, Gallagher J S and Kell G S 1984 NBS/NRC Steam Tables: Thermodynamic and Transport Properties and Computer Programs for Vapor and Liquid States of Water in SI Units (Washington, DC: Hemisphere) p 271276
[15] Scala A, Starr F W, La Nave E, Sciortino F and Stanley H E 2000 Nature 406 166
[16] Chaplin M 2020 Anomalous properties of water www.lsbu.ac.uk/water/amniiies.html
[17] Hemmer P C and Stell G 1970 Phys. Rev. Lett. 24 1284
[18] Stell G and Hemmer P C 1972 J. Chem. Phys. 56 4274
[19] Debenedetti P G, Raghavan V S and Borik S S 1991 J. Phys. Chem. 95 4540
[20] Ryzhov V N, Tareyeva E E, Fomin Yu D and Tsiok E N 2020 Phys.-Usp. 63 5
[21] Fomin Yu D, Tsiok E N, Ryzhov V N and Brazhkin V V 2019 Fluid Phase Equilib. 498 45–50
[22] Fomin Yu D, Tsiok E N, Ryzhov V N and Brazhkin V V 2019 J. Mol. Liq. 287 110992
[23] Hujo W, Japes B S, Rana V K, Chakravarty C and Molineoro V 2011 J. Stat. Phys. 145 293–312
[24] Japes B S, Nayar D, Dhabal D, Molineoro V and Chakravarty C 2012 J. Phys.: Condens. Matter 24 284116
[25] Molineoro V and Moore E B 2009 J. Phys. Chem. B 113 4008–16
[26] Vasilish V, Saw S and Sastry S 2011 Nat. Phys. 7 549–53
[27] Vasilish V, Mathew J, Sengupta S and Sastry S 2014 J. Chem. Phys. 114 124501
[28] Dhabal D, Chakravarty C, Molineoro V and Kashyap H K 2016 J. Chem. Phys. 145 214502
[29] Poole P H, Sciortino F, Essmann E and Stanley H E 1992 Nature 360 324–8
[30] Stillinger F H and Weber T A 1985 Phys. Rev. B 31 5262
[31] Savvatimskiy A I 1995 Carbon 43 1115–42
[32] Fomin Yu D and Brazhkin V V 2019 Carbon 157 767–78
[33] Fomin Yu D, Ryzhov V N, Klumov B A and Tsiok E N 2014 J. Chem. Phys. 141 034508
[34] Ranieri U, Giura P, Gorelli F A, Santoro M, Klotz S, Gillet P, Paolalini L, Koza Z M and Bove L E 2016 J. Phys. Chem. 120 9051–9
[35] Etienne J P and McDonald I R 2013 Theory of Simple Liquids (New York: Elsevier)
[36] Rapaport D C 1995 The Art of Molecular Dynamics Simulation (Cambridge: Cambridge University Press)
[37] Fomin Yu D 2019 J. Phys. Chem. Liq. 57 67–74
[38] Fomin Yu D 2018 Mol. Phys. 115 2786–92
[39] Plimpton S 1995 J. Comp. Phys. 117 1–19
[40] Jedlovszky P, Garberoglio G and Vallauri R 2011 Phys. Chem. Chem. Phys. 13 19823–9
[41] Khusnutdinoff R M 2016 Colloid J. 78 225–34
[42] Hosokawa et al 2003 J. Phys.: Condens. Matter 15 L623–9
[43] Berendsen H J C, Grigera J R and Straatsma T P 1987 J. Phys. Chem. 91 6269–71
[44] Fomin Yu D, Ryzhov V N, Tsiok E N and Brazhkin V V 2015 Sci. Rep. 5 14234
[45] Yang C, Brazhkin V V, Dove M T and Trachenko K 2015 Phys. Rev. Lett. 115 215502
[46] Sanz E, Vega C, Abascal J L F and MacDowell L G 2004 Phys. Rev. Lett. 92 255701
[47] Vega C, Abascal J L F, Sanz E, MacDowell L G and McBride C 2005 J. Phys.: Condens. Matter 17 S3283–8
[48] Guissani Y and Guillot B 1993 J. Chem. Phys. 98 8221
[49] Brazhkin V V, Lyapin A G, Ryzhov V N, Trachenko K, Fomin Yu D and Tsiok E N 2012 Phys.–Usp. 55 1061–79
[50] Brazhkin V V, Fomin Yu D, Lyapin A G, Ryzhov V N and Trachenko K 2012 Phys. Rev. E 85 031203
[51] Brazhkin V V, Fomin Yu D, Lyapin A G, Ryzhov V N, Tsiok E N and Trachenko K 2013 Phys. Rev. Lett. 111 145901
[52] Fomin Yu D, Ryzhov V N, Tsiok E N, Brazhkin V V and Trachenko K 2016 J. Phys.: Condens. Matter 28 43LT01
[53] Fomin Yu D, Ryzhov V N, Tsiok E N, Proctor J E, Prescher C, Prakapenka V B, Trachenko K and Brazhkin V V 2018 J. Phys.: Condens. Matter 30 134003
[54] Yang C, Dove M T, Brazhkin V V and Trachenko K 2017 Phys. Rev. Lett. 118 215502