Colloid Journal 2017 vol.79 N1, pages 26-34

Surface tension of water droplets upon homogeneous droplet nucleation in water vapor

Galimzyanov B., Mokshin A.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2017, Pleiades Publishing, Ltd.A method has been proposed for determining interfacial free energy from the data of molecular dynamics simulation. The method is based on the thermodynamic integration procedure and is distinguished by applicability to both planar interfaces and those characterized by a high curvature. The workability of the method has been demonstrated by the example of determining the surface tension for critical nuclei of water droplets upon condensation of water vapor. The calculation has been performed at temperatures of 273–373 K and a pressure of 1 atm, thus making it possible to determine the temperature dependence of the surface tension for water droplets and compare the results obtained with experimental data and the simulation results for a “planar” vapor–liquid interface.

http://dx.doi.org/10.1134/S1061933X17010057

References

[1] Frenkel’, Ya.I., Kineticheskaya teoriya zhidkostei (Kinetic Theory of Liquids), Leningrad: Nauka, 1975.
[2] Kashchiev, D., Nucleation: Basic Theory with Applications, Oxford: Butterworth-Heinemann, 2000.
[3] Mokshin, A.V., Teor. Mat. Fiz., 2015, vol. 183, p. 3.
[4] Fokin, V.M., Zanotto, E.D., Yuritsyn, N.S., and Schmelzer, J.W.P., J. Non-Cryst. Solids, 2006, vol. 352, p. 2681.
[5] Zubarev, D.N., Neravnovesnaya statisticheskaya termodinamika (Nonequilibrium Statistical Thermodynamics), Moscow: Mir, 1980.
[6] Zubarev, D.N. and Morozov, V.G., Statistical Mechanics of Nonequilibrium Processes. Vol. 1. Basic Concepts. Kinetic Theory, Berlin: Academic, 1996.
[7] Fokin, V.M., Zanotto, E.D., and Schmelzer, J.W.P., J. Non-Cryst. Solids, 2003, vol. 321, p. 52.
[8] Tovbin, Yu.K., Russ. J. Phys. Chem. A, 2010, vol. 84, p. 1717.
[9] Tovbin, Yu.K. and Rabinovich, A.B., Izv. Akad. Nauk, Ser. Khim., 2010, vol. 4, p. 663.
[10] Skripov, V.P., Metastabil’naya zhidkost’ (Metastable Liquid), Moscow: Nauka, 1972.
[11] Zheligovskaya, E.A. and Malenkov, G.G., Zh. Strukt. Khim., 2005, vol. 46, p. 284.
[12] Malenkov, G.G., Zh. Strukt. Khim., 2006, vol. 47, p. 5.
[13] Shevkunov, S.V., Zh. Eksp. Teor. Fiz., 2009, vol. 136, p. 282.
[14] Shevkunov, S.V., Zh. Eksp. Teor. Fiz., 2009, vol. 135, p. 510.
[15] Malenkov, G.G., Colloid J., 2010, vol. 72, p. 653.
[16] Malenkov, G.G., Zh. Strukt. Khim., 2013, vol. 54, p. 258.
[17] Shevkunov, S.V., High Temperature, 2013, vol. 51, p. 79.
[18] Molinero, V. and Moore, E.B., J. Phys. Chem. B, 2009, vol. 113, p. 4008.
[19] Moore, E.B. and Molinero, V., Nature (London), 2011, vol. 479, p. 506.
[20] Mokshin, A.V. and Galimzyanov, B.N., J. Phys. Chem. B, 2012, vol. 116, p. 11959.

[21] Zipoli, F., Laino, T., Stolz, S., Martin, E., Winkelmann, C., et al., J. Chem. Phys., 2013, vol. 139, p. 094501.

[22] Stanley, H.E. and Teixeira, J., J. Chem. Phys., 1980, vol. 73, p. 3404.

[23] Biscay, F., Ghoufi, A., Lachet, V., and Malfreyt, P., J. Phys. Chem., 2011, vol. 115, p. 8670.

[24] Irving, J.H. and Kirkwood, J.G., J. Chem. Phys., 1950, vol. 18, p. 817.

[25] Kirkwood, J.G. and Buff, F.P., J. Chem. Phys., 1949, vol. 17, p. 338.

[26] Stillinger, F. and Weber, T.A., Phys. Rev. B, 1985, vol. 31, p. 5262.

[27] Frenkel, D. and Smit, B., Understanding Molecular Simulation: From Algorithms to Applications, San Diego: Academic, 2007.

[28] Mokshin, A.V., Zabegaev, S.O., and Khusnutdinov, R.M., Phys. Solid State, 2011, vol. 53, p. 570.

[29] Khusnutdinov, R.M. and Mokshin, A.V., JETP Lett., 2014, vol. 100, p. 39.

[30] Mokshin, A.V., Khusnutdinov, R.M., Novikov, A.G., Blagoveshchenskii, N.M., and Puchkov, A.V., Zh. Eksp. Teor. Fiz., 2015, vol. 148, p. 947.

[31] Mokshin, A.V. and Galimzyanov, B.N., J. Chem. Phys., 2014, vol. 140, p. 024104.

[32] Mokshin, A.V., Galimzyanov, B.N., and Barrat, J.-L., Phys. Rev. E: Stat. Phys., Plasmas, Fluids, Relat. Interdiscip. Top., 2013, vol. 87, p. 062307.

[33] Moody, M.P. and Attard, P., Phys. Rev. Lett., 2013, vol. 91, p. 056104.

[34] Schmelzer, J. and Mahnke, R., J. Chem. Soc., Faraday Trans., 1986, vol. 82, p. 1413.

[35] Tolman, R.S., J. Chem. Phys., 1949, vol. 17, p. 333.

[36] Vega, C. and De Miguel, E., J. Chem. Phys., 2007, vol. 126, p. 154707.

[37] White, H. and Sengers, J.V., Release on the Surface Tension of Ordinary Water Substance, Int. Association for the Properties of Water and Steam (IAPWS). 12 Int. Conf. on Properties of Water and Steam, New York: Begell House, 1995.

[38] Ismail, A.E., Grest, G.S., and Stevens, M.J., J. Chem. Phys., 2006, vol. 125, p. 014702.

[39] Robinson, G.W., Singh, S., Zhu, S.B., and Evans, M.W., Water in Biology, Chemistry and Physics: Experimental Overviews and Computational Methodologies, Singapore: World Scientific, 1996.

[40] Chen, F. and Smith, P.E., J. Chem. Phys., 2007, vol. 126, p. 221101.

[41] Alder, B.J. and Wainwright, T.E., J. Chem. Phys., 1957, vol. 27, p. 1208.