VERSIONS OF THE THERMODYNAMIC PERTURBATION THEORY AND THE CHOICE OF THE OPTIMAL VERSION FOR CALCULATIONS OF THERMODYNAMIC PROPERTIES OF SUBSTANCES

Yu. A. Bogdanova, I. V. Maklashova, and T. D. Tret'yakova

National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation

Abstract: The basic principles of the perturbation theory for calculating the thermodynamic properties of pure systems have been reviewed. The versions of various authors have been analyzed to select the most accurate one. The verification has been carried out by comparing the results of calculations of the thermodynamic parameters of pure system with the interaction potential Exp-6, isothermal compression of helium with the Lennard-Jones potential, and the parameters of the state of liquid aluminum with Morse potential with Monte-Carlo simulation and experimental data.

Keywords: perturbation theory; intermolecular interaction potential; equation of state; fluids; isothermal compression

DOI: 10.30826/CE19120117

Acknowledgments

The work was supported by the Russian Science Foundation (project No. 16-19-00188).

References

1. Henderson, D., and J. A. Barker. 1967. Perturbation theory and equation of state for fluids. II. A successful theory of liquids. *J. Chem. Phys.* 47(11):4714–4721. doi: 10.1063/1.1701689.
2. Weeks, J. D., D. Chandler, and H. C. Andersen. 1971. Role of repulsive forces in determining the equilibrium structure of simple liquids. *J. Chem. Phys.* 54:5237–5247. doi: 10.1063/1.1674820.
3. Kang, H. S., C. S. Lee, T. Ree, and F. H. Ree. 1985. A perturbation theory of classical equilibrium fluids. *J. Chem. Phys.* 82(1):414–423. doi: 10.1063/1.448762.
4. Carnahan, N. F., and K. E. Starling. 1969. Equation of state for nonattracting rigid spheres. *J. Chem. Phys.* 51: 635-636. doi: 10.1063/1.1672048.
5. Leonard, P. J., D. Henderson, and J. A. Barker. 1970. Perturbation theory and liquid mixtures. *T. Faraday Soc.* 66:2439–2452. doi: 10.1039/TF9706602439.
6. Rogers, B. L., and J. M. Prausnitz. 1971. Calculation of high-pressure vapour–liquid equilibriums with a perturbed hard-sphere equation of state. *T. Faraday Soc.* 67:3474–3483. doi: 10.1039/TF9716703474.
7. Weeks, J. D., D. Chandler, and H. C. Andersen. 1971. Relationship between the hard-sphere fluid and fluids with realistic repulsive forces. *Phys. Rev. A* 4(4):1597–1607. doi: 10.1103/PhysRevA.4.1597.
8. Weeks, J. D., D. Chandler, and H. C. Andersen. 1971. Perturbation theory of the thermodynamic properties of simple liquids. *J. Chem. Phys.* 55(11):5422–5423. doi: 10.1063/1.1675700.
9. Bratkovsky, A. M., V. G. Vaks, and A. V. Trefilov. 1983. On the accuracy of the liquid theory approximate methods for the description of liquid metal thermodynamics. *J. Phys. F. Met. Phys.* 13:2517–2542. doi: 10.1103/PhysRevB.96.024203.
10. Kahl, G., and J. Hafner. 1985. A blip-function calculation of the structure of liquid binary alloys. *J. Phys. F* 15(8):1627–1638. doi: 10.1088/0305-4608/15/8/003.
11. Ng, D. A., and M. Silbert. 1988. WCA studies of the partial structure factors of liquid binary alloys: Application to Al–Mg*. *J. Phys. Chem.* 156:663–669. doi: 10.1524/zpch.1988.156.Part_2.663.
12. Dubinin, N. E., A. A. Yur'ev, and N. A. Vatolin. 1993. Primenenie metoda WCA dlya rascheta termodinamicheskikh svoystv dvukhkomponentnykh metallicheskikh rasplavov [Application of WCA-method to calculate the thermodynamic properties of liquid binary metal alloys]. *Dokl. Akad. Nauk* 332(3):325–327.
13. Dubinin, N. E., A. A. Yuryev, and N. A. Vatolin. 2011. Straightforward calculation of the WCA entropy and internal energy for liquid metals. *Thermochim. Acta* 518(1-2):9–12. doi: 10.1016/j.tca.2011.01.041.
14. Byers-Brown, W., and T. V. Horton. 1988. Hard-sphere perturbation theory for classical fluids to high densities. *Mol. Phys.* 63(1):125–138. doi: 10.1080/00268978800100101.

15. Vargaftik, N. B. 1972. *Spravochnik po teplofizicheskim svoystvam gazov i zhidkostey* [Handbook of the thermophysical properties of gases and liquids]. Moscow: Nauka. 720 p.
16. Tsiklis, D. S. 1977. *Plotnye gasy* [Dense gases]. Moscow: Khimiya. 168 p.
17. Fried, L. E., and W. M. Howard. 1998. An accurate equation of state for the exponential-6 fluid applied to dense supercritical nitrogen. *J. Chem. Phys.* 109(17):7338–7348. doi: 10.1063/1.476520.
18. Selezenev, A. A., A. Yu. Aleynikov, N. S. Gantchuk, *et al.* 2003. SageMD: Molecular-dynamic software package to study properties of materials with different models for interatomicinteractions. *Comp. Mater. Sci.* 28:107–124. doi: 10.1016/S0927-0256(03)00101-0.
19. Gubin S. A., I. V. Maklashova, and K. S. Melnikova. 2012. Teplofizicheskie i mekhanicheskie svoystva kompozita iz alyuminiya i oksida alyuminiya na osnove modeli additivnogo smesheniya [The thermophysical and mechanical properties of a composite of aluminum and aluminum oxide-based additive mixing model]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 5(5):297–301.
20. Murnagan, F. D. 1944. The compressibility of media under extreme pressures. *P. Natl. Acad. Sci. USA* 30(9):244–248. doi: 10.1073/pnas.30.9.244.
21. Vaboya, S. N., and G. C. Kennedy. 1970. Compressibility of 18 metals to 45 kbar. *J. Phys. Chem. Solids* 31(10):2329–2345. doi: 10.1016/0022-3697(70)90247-7.
22. Syassen, K., and W. B. Holzapfel. 1978. Isotermal compression of Al and Ag to 120 kbar. *J. Appl. Phys.* 49:427–4430. doi: 10.1063/1.325497.
23. Litygina, L. M., Z. V. Malyushtskaya, T. A. Pashkina, and S. S. Kabalkina. 1982. Isotermal compression of Al to 10 GPa at 673 K. *Phys. Status Solidi A* 69(2):K147–K150. doi: 10.1002/pssa.2210690247.
24. Dewaele, A., P. Loubeyre, and M. Mezouar. 2004. Equations of state of six metals above 94 GPa. *Phys. Rev. B* 70:094112-1–094112-8. doi: 10.1103/PhysRevB.70.094112.

Received December 25, 2018

Contributors

Bogdanova Youlia A. (b. 1983) — assistant, Department of Chemical Physics No. 4, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation; bogdanova.youlia@bk.ru

Maklashova Irina V. (b. 1975) — senior teacher, Department of Chemical Physics No. 4, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation; ivmaklashova@mephi.ru

Tret'yakova Tat'yana D. (b. 1997) — student, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation; tutimaggie1@gmail.com