APPLICATION PERTURBATION THEORY FOR CALCULATION OF THE THERMODYNAMIC PROPERTIES OF METALS

Yu. A. Bogdanova, S. A. Gubin, I. V. Maklashova, A. V. Kudinov, and I. N. Melnikov

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

Abstract: Application of the equation of state based on perturbation theory is demonstrated on calculating the properties of condensed aluminum and copper during isothermal compression. For a description of intermolecular interactions in metals, Morse pair potential is used. The calculation results are in good agreement with experimental data and calculations based on the described in the literature empirical and analytical equations of state. Thus, the equation of state developed on the basis of perturbation theory and using the corresponding intermolecular interaction potential is a reliable universal tool for the calculation of the thermodynamic properties of gas (fluid) systems and condensed matter physics and allows one to analyze changes in the atomic structure of the matter.

Keywords: perturbation theory; intermolecular interaction potential Morse; thermodynamic parameters of state; radial distribution function; isothermal compression

Acknowledgments

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

References

1. Gubin, S. A., I. V. Maklashova, A. A. Selezenev, *et al.* 2014. Molecular dynamics simulation and visualization of melting aluminum crystal in shock wave. *Scientific Visualization* 6(5):14–23.
2. Gubin, S. A., I. V. Maklashova, A. A. Selezenev, and S. A. Kozlova. 2015. Molecular-dynamics study melting aluminum at high pressures. *Physics Procedia* 72: 338–341.
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.
4. Byers-Brown, W., and T. V. Horton. 1988. Hard-sphere perturbation theory for classical fluids to high densities. *Mol. Phys.* 63(1):125–138.
5. Ross, M. 1979. A high-density fluid-perturbation theory based on an inverse 12th-power hard-sphere reference system. *J. Chem. Phys.* 71(4):1567–1571.
6. Victorov, S. B., and S. A. Gubin. 2016. *Termodinamicheskoe modelirovanie slozhnykh khimicheskikh sistem pri vysokikh davleniyakh i temperaturakh* [Thermodynamic modeling of complicated chemical systems at high pressures and temperatures]. Moscow: NRNO MEPhI. 128 p.
7. 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(12):5237–5247.
8. 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.
9. 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.
10. 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 Metal Phys.* 13(12):2517–2542.
11. Kahl, G., and J. Hafner. 1985. A blip-function calculation of the structure of liquid binary alloys. *J. Phys. F Metal Phys.* 15(8):1627–1638.
12. 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(2):663–669.
13. 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.
14. Dubinin, N. E., A. A. Yuryev, and N. A. Vatolin. 2011. Straightforward calculation of the WCA entropy and internal energy for liquid metals. *Thermochimica Acta* 518(1-2):9–12.
15. Victorov, S. B., H. El-Rabii, S. A. Gubin, I. V. Maklashova, and Yu. A. Bogdanova. 2010. An accurate equation-of-state model for thermodynamic calculations of chemically reactive carbon-containing systems. *J. Energ. Mater.* 28(sup1):35–49.
16. Bogdanova, Y. A., S. A. Gubin, S. B. Viktorov, V. A. Shargatov, and A. V. Lyubimov. 2010. Application of perturbation theory to a mixture of hydrogen atoms and molecules with the Morse intermolecular interaction potential. *Russ. Phys. J.* 53(3):243–256.
17. Bogdanova, Yu. A., S. A. Gubin, A. A. Anikeev, and S. B. Victorov. 2016. Application of a theoretical model of state equation for calculation of N_2, O_2, and CO_2 shock adiabatic curves. *Russ. Phys. J.* 59(2):190–196.

18. *Selezenev A. A., Aleynikov A. Yu., N. S. Gantchuk, et al.* 2003. Sage MD: Molecular-dynamic software package to study properties of materials with different models for interatomic interactions. *Comput. Mater. Sci.* 28:107–124.
19. Throop, G. J., and R. J. Bearman. 1965. Radial distribution functions for mixtures of hard spheres. *J. Chem. Phys.* 42:2838–2843.
20. Leonard, P. J., D. Henderson, and J. A. Barker. 1971. Calculation of the radial distribution function of hard-sphere mixtures in the Percus–Yevick approximation. *Molec. Phys.* 21(1):107–111.
21. Lebowitz, J. L. 1964. Exact solution of generalized Percus–Yevick equation for a mixture of hard sphere. *Phys. Rev.* 133:A895.
22. Bogdanova, Y. A., S. A. Gubin, S. B. Viktorov, A. V. Lyubimov, and V. A. Shargatov. 2010. Calculation of distribution functions for two-component rigid-sphere molecules of a fluid. *Russ. Phys. J.* 53(2):114–122.
23. Smith, W. R., and D. Henderson. 1970. Analytical representation of the Percus–Yevick hard-sphere radial distribution function. *Molec. Phys.* 19(3):411–415.
24. Waseda, Y., and K. Suzuki. 1972. Characteristics of soft core in pair potential and static structure in liquid metals. *Science Reports of the Research Institutes, Tohoku University. Ser. A, Physics, chemistry and metallurgy* 24:139–184.
25. Waseda, Y., and S. Tamaki. 1975. The structures of 3d-transition metals in the liquid state. *Phil. Mag.* 32(2):273–281.
26. Bogdanova, Y. A., S. A. Gubin, S. B. Victorov, and T. V. Gubina. 2015. A theoretical model of the equation of state of a two-component fluid with the exp-6 potential based on perturbation theory. *High Temp.* 53(4):481–490.
27. 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* 5:297–301.
28. Murnagan, F. D. 1944. The compressibility of media under extreme pressures. *Proc. Natl. Acad. Sci.* 30(9):244–248.
29. Vaboya, S. N., and G. C. Kennedy. 1970. Compressibility of 18 metals to 45 kbar. *J. Phys. Chem. Solids* 31(10):2329–2345.
30. Mao, H. K., and P. M. Bell. 1978. Specific volume measurement of Cu, Mo, Pd and Ag and calibration of the ruby R1 fluorescence pressure gouge from 0.06 to 1 Mbar. *J. Appl. Phys.* 49(6):3276–3283.
31. Syassen, K., and W. B. Holzapfel. 1978. Isotermal compression of Al and Ag to 120 kbar. *J. Appl. Phys.* 49:4427–4430.

Received December 29, 2016

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

Gubin Sergey A. (b. 1945) — professor, head of department, Department of Chemical Physics No. 4, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation; gubin_sa@mail.ru

Maklashova Irina V. (b. 1975) — senior lecturer, 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

Kudinov Andrey V. (b. 1996) — student, Department of Chemical Physics No. 4, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation; swen379@gmail.com

Melnikov Igor N. (b. 1996) — student, Department of Chemical Physics No. 4, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation; 12ewt@mail.ru