

NUMERICAL THERMODYNAMIC ANALYSIS OF ALLOYS FOR PLASMA ELECTRONICS AND ADVANCED TECHNOLOGIES

V.V. Kuzenov^{1,2}, S.V. Ryzhkov¹, V.V. Shumaev¹

¹*Bauman Moscow State Technical University, Moscow, Russia;*

²*A.Yu. Ishlinsky Institute for Problems in Mechanics RAS, Moscow, Russia*

E-mail: kuzenov@ipmnet.ru; svryzhkov@bmstu.ru; shumaev@student.bmstu.ru

Thermodynamic properties (pressure, specific internal energy and entropy) of the ionized gas mixture are obtained on the basis of the Thomas-Fermi theory and Saha model. The calculations was made for the lithium-indium alloy (Li + 10% In), which has various applications in plasma electronics and technology.

PACS: 52.25.Kn, 31.15.Bs

INTRODUCTION

Nowadays it is explored the possibility of combination of two nuclear power production methods and the possibility of creation fission-fusion hybrid reactors. Fusion devices can be used for the destruction of long-lived radioactive wastes from fission reactors. In the nearest future perspective technologies and high-energy-density systems, in particular, neutron and proton sources, will be important for the material science, analysis and non-destructive control, medical isotope production, chemical waste destruction, personnel training and etc.

However, the hybrid way of fusion exists. It is known as magneto-inertial fusion (MIF) [1 - 4], where are used as drivers the capacitor and inductive stores (electrodynamic method), magneto-explosive generators, explosive charges (explosive method) and the energy of the compressed gas (gas dynamics method). We consider the compression and heating of plasmoid which is confined by the ultra-strong external magnetic field, high-speed plasma jets and laser beams with high-energy impulse. Ultra-strong magnetic fields reduce electronic thermal losses and provide sufficient plasma confinement.

The calculation of thermal processes in MIF systems, powerful and compact fusion neutron sources and experimental prototypes of perspective systems and devices based on the fusion plasma in the magnetic field requires to develop methods of computational and theoretical justification of the energy efficiency and optimization of alternative systems and perspective ways of power production. Moreover, it is important to determine magneto-inertial regimes for perspective devices: fusion reactors with plasma (argon or xenon) liner and neutron generators and to optimize these regimes considering specifications which allow creating economically viable industrial plants.

The critical part of magneto-inertial system for plasma confinement is the final stage of compression where the corresponding isolation and plasma confinement, rotational speed for hydrodynamic stability are necessary. Authors have developed the two-dimensional radiation-magneto gas dynamics code PLUM which is the part of the nonstationary instruments and codes for fusion applications (NICA) and includes radiation transport in multi group diffusion approach and gas dynamics with dynamic adaptive grid and finite difference scheme with the increased order of accuracy, and also the influence on hydrodynamics of plasma by the ener-

gy release [5]. The possibility of the hydrodynamics instability suppression with the external magnetic field is represented in papers [6 - 8].

The important problem for the hydrodynamics calculations of processes in plasma is to determine its thermodynamic (the pressure, specific internal energy and entropy) and transport properties (electrical conductivity and heat conductivity coefficients, optical properties). Authors have developed the computational code for evaluation the thermodynamic properties of ionized gases mixture in the magnetic field based on the Thomas-Fermi (TF) model. It is called TERMAG [9, 10]. Nowadays the code is supplemented with ionization equilibrium model (Saha model) which will allow expanding the region of the code applicability to lower temperatures and densities.

The TF theory has different applications [11 - 13]. The Thomas-Fermi-Firsov energy transfer calculations are used for the analysis of the emission of electrons from a metal surface [14], the Thomas-Fermi von Weizsacker theory is used to investigate the properties of metal surfaces (the work function and surface energy) [15] and it can be also used in the theory of metallic clusters [16]. The TF screening length is used in the isolated ferroelectric domain walls analysis [17].

The analysis we made are related to the question of lithium and indium applicability in fusion [18], electrical engineering [19] and electronic [20] systems.

1. THERMODYNAMIC AND GAS-DYNAMIC ASPECTS OF PLASMA TECHNOLOGIES

In high-energy-density systems, e.g. neutron and proton sources based on inertial plasma confinement it is important to compress the target in such a way that only its central part reaches the temperature of the ignition while the rest parts of the fuel is cold. This mode can be characterized by the minimum driver energy because the energy is used only for compressing the fuel to a high density [21]. To provide such energy efficient fusion burning, it is necessary to compress the core of the target in the isentropic regime to the value $\rho R > 1 \text{ g/cm}^2$, where ρ is the plasma density; R is the radius of the target. Note that in the presence of the strong magnetic field typical for MIF devices this condition changes. For the cylindrical target it looks like [22]:

$$\left. \begin{aligned} T &\geq 7 \dots 10 \text{ keV} \\ B \cdot R &\geq (4.5 \dots 6.5) \cdot 10^5 \text{ G} \cdot \text{cm} \end{aligned} \right\},$$

where B is the magnetic induction.

The common formulation of the computational problem for the MIF processes requires taking into consideration the influence of the external magnetic field with induction to 10^4 T [23, 24] on the plasma thermodynamic and transport properties. Evaluations have been made by authors show that the magnetic field of such induction influences only the transport properties of plasma but it does not change the shape of internal atom or ion shells [25].

It is required to consider the processes of the isentropic compression of the target by converging shock waves together with the thermal and caloric equations of state for the substance on different stages including the stage of the high compression i.e. in a wide range of densities (from gas-like up to $10^3 \dots 10^4$ g/cm³) and temperatures (from a few thousands K to a hundred millions K).

Nowadays the obtaining equations of state for substance in such wide range of parameters are connected with the problem of joining the solutions. The TF model is rather simple and precise. It can be used in the area of high temperatures and densities (temperatures $T > 10^5$ K, densities of solid body and higher) [26, 27]. The Saha model is used for lower temperatures and densities [26 - 28].

Methods for calculating thermodynamic properties (the pressure, specific internal energy and entropy) of ionized gases mixtures are described in the following papers: for the TF model [25 - 27, 29], for Saha equations [26 - 28, 30]. Authors performed calculations by the TF model, but values of thermodynamic functions according the Saha model were taken from [30].

2. CALCULATION RESULTS

The graphical correlation between temperature and pressure P , specific internal energy E and entropy S for mixture Li + 10% In at average densities $\rho = 2.94 \cdot 10^{-6}$, $2.94 \cdot 10^{-4}$, and $2.94 \cdot 10^{-2}$ g/cm³ obtained by computational code TERMAG (TF model) and Saha model literature data are shown in the Figs. 1,a-c. Note, that the smooth conjugation of the calculation results according these models haven't been carried out in this paper.

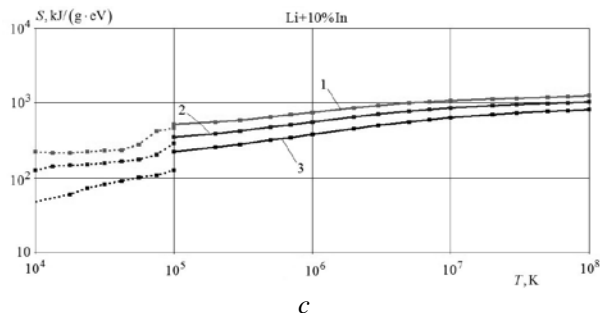
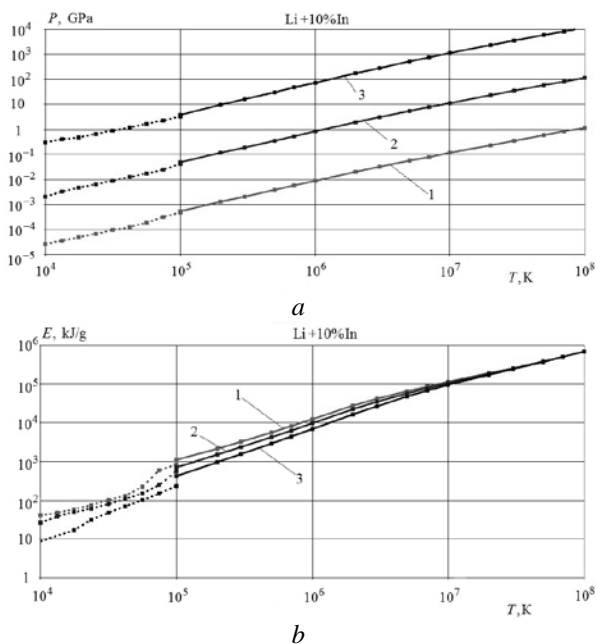


Fig. 1. Thermodynamic functions of the Li + 10% In mixture depending on the temperature calculated by Saha (dotted line) and Thomas-Fermi (solid line) models: the pressure (a); specific internal energy (b); specific entropy (c). The average density of mixture: 1 - $2.94 \cdot 10^{-6}$ g/cm³; 2 - $2.94 \cdot 10^{-4}$ g/cm³; 3 - $2.94 \cdot 10^{-2}$ g/cm³

With increasing average density increases the pressure, but the specific internal energy and entropy decrease. A decrease in the average density causes the decrease in the difference between the results obtained by the TF model and Saha model at $T = 10^5$ K. This can be explained as the increase of the plasma ideality so the accuracy of Saha equations also increases (the TF model is not as sensitive to the changes in the density).

The Saha and TF models describe the transition area of thermodynamics parameters $10^{-7} < \rho < 10^{-1}$ g/cm³, $10^3 < T < 10^6$ K. Figs. 2,a-c represents thermodynamic functions $P(T)$, $E(T)$, $S(T)$ in this region of parameters.

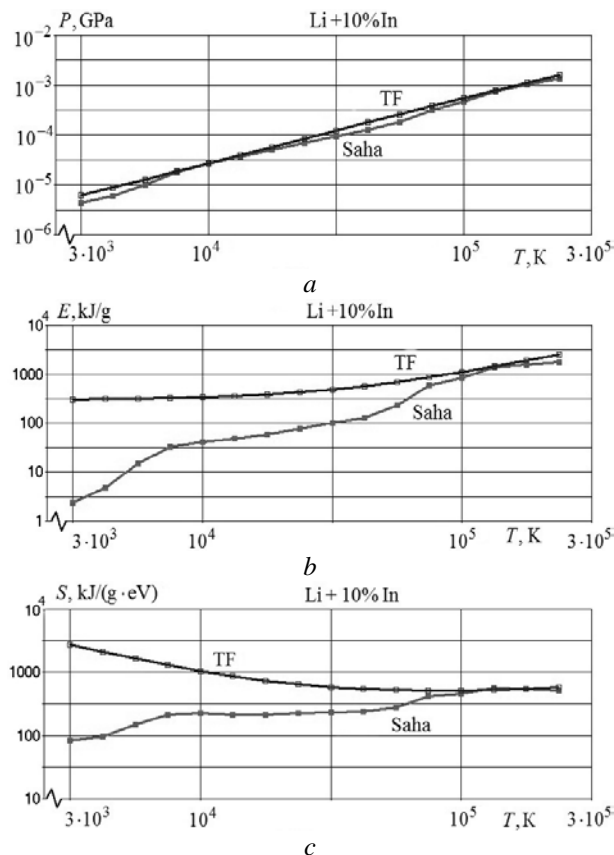


Fig. 2. Thermodynamic functions of the Li + 10% In mixture depending on the temperature in the region where both models can work. The average density of mixture is $2.94 \cdot 10^{-6}$ g/cm³

On the Figs. 2,a-c. TF model represents a smooth curve, because this model averages the effects of the atomic shell structure. Fig. 2,a shows two areas of good result agreement: at $T \sim 10^4$ and $\sim 10^5$ K. At the same time Fig. 2,b and c show that the result agreement grows when the temperature increases. It is known that the accuracy of the TF increases with temperature [26, 29]. Therefore the increase in the model results difference at $T \sim 3 \cdot 10^5$ K can be explained as the fact that the Saha model reaches its boundary of the applicability area. The difference between these model results at $T \sim 10^3 \dots 10^4$ K is intolerably huge. This happens, because the thermodynamic properties, obtained by the TF model, are inaccurate in this temperature range [29].

CONCLUSIONS

It is necessary to solve the systems of magnetohydrodynamics equations including Maxwell's equations and wide-range equation of state for the calculation of thermal physical processes in perspective high-energy-density systems like magneto-inertial fusion devices. Wide-range equation of state can be found by conjugation the solutions of the TF model for rather high temperatures T and densities ρ and the Saha model for low T and ρ .

This paper illustrates the calculation results of the ionized gas mixture thermodynamic properties (the pressure, specific internal energy and entropy) on the basis of the TF theory and Saha equations. These calculations was made for the lithium-indium alloy (Li+10% In) for temperatures $T = 3 \cdot 10^3 \dots 10^8$ K and densities $\rho = (10^{-6} \dots 10^{-2})$ g·cm⁻³ by the computational code for evaluation the thermodynamic properties of ionized gases mixture in the magnetic field based on the TF model (TERMAG) and the published data on the Saha model. Analysis we made is related to the question of lithium and indium application in energy (fusion device first wall), electric (lithium-indium alloy compound in batteries) and electronics (indium layer or additive on the lithium base) systems. The TF model can be also used for energy transfer calculations in the analysis of the electron emission from a metal surface, to investigate the properties of metal surfaces (the work function and surface energy), and also in the theory of metallic clusters.

This work was supported by the Ministry of Education and Science of the Russian Federation (Project № 13.79.2014/K).

REFERENCES

1. S.V. Ryzhkov. Current state, problems, and prospects of thermonuclear facilities based on the magneto-inertial confinement of hot plasma // *Bulletin of the Russian Academy of Sciences. Physics*. 2014, v. 78, № 5, p. 456-461.
2. V.V. Kuzenov, S.V. Ryzhkov. Numerical modeling of magnetized plasma compressed by the laser beams and plasma jets // *Problems of Atomic Science and Technology*. 2013, №1 (83), p. 12-14.
3. V.V. Kuzenov, S.V. Ryzhkov. Regimes of Heating and Compression in Magneto-Inertial Fusion // *Proc. of the 15th International Heat Transfer Conference*. 2014, IHTC15-9662.
4. I.Yu. Kostyukov, S.V. Ryzhkov. Magneto-Inertial Fusion with Laser Compression of a Magnetized Spherical Target // *Plasma Physics Reports*. 2011, v. 37, № 13, p. 1092-1098.
5. V.V. Kuzenov, S.V. Ryzhkov. Evaluation of hydrodynamic instabilities in inertial confinement fusion target in a magnetic field // *Problems of Atomic Science and Technology*. 2013, № 4 (86), p. 103-107.
6. S.V. Ryzhkov. The behavior of a magnetized plasma under the action of laser with high pulse energy // *Problems of Atomic Science and Technology. Series «Plasma Electronics and New Methods of Acceleration»*. 2010, № 4, p. 105-110.
7. R. Samtaney. Suppression of the Richtmyer-Meshkov instability in the presence of a magnetic field // *Phys. Fluids*. 2003, v. 15, L53.
8. T. Sano, T. Inoue, K. Nishihara. Critical magnetic field strength for suppression of the Richtmyer-Meshkov instability in plasmas // *Phys. Rev. Lett*. 2013, v. 111, p. 205001.
9. V.V. Kuzenov, S.V. Ryzhkov, V.V. Shumaev. Application of Thomas-Fermi model to evaluation of thermodynamic properties of magnetized plasma // *Problems of Atomic Science and Technology*. 2015, № 1, p. 97-99.
10. V.V. Kuzenov, V.V. Shumaev. Description of the thermodynamic properties of plasma in Saha and Thomas-Fermi models // *Applied Physics*. 2015, №2, p. 32-36.
11. L.Z. Zhang, Z.C. Wang. Analytical solution of the Boltzmann-Poisson equation and its application to MIS tunneling junctions // *Chinese Physics B*. 2009, v. 18, № 7, p. 2975-2980.
12. B. Grandidier, D. Stievenard, D. Deresmes, et al. Influence of electron irradiation induced defects on the current-voltage characteristics of a resonant tunneling diode // *Materials Science Forum. Proceedings of the 17th International Conference on Defects in Semiconductors*. 1994, v. 143-4 (pt. 3), p. 1553-1558.
13. C.L. Fernando, W.R. Frensley. Hybrid quantum-classical model for transport in tunneling heterostructures // *Proceedings of the IEEE Cornell Conference on Advanced Concepts in High Speed Semiconductor Devices and Circuits*. 1993, p. 152-158.
14. D.E. Harrison Jr., C.E. Carlston, G.D. Magnuson. Kinetic emission of electrons from monocrystalline targets // *Phys. Rev*. 1965, v. 139, № 3A, p. A737-A745.
15. A. Chizmeshya, E. Zaremba. Second-harmonic generation at metal surfaces using an extended Thomas Fermi von Weizsacker theory // *Physical Review B*. 1988, v. 37, № 6, p. 2805-2811.
16. E. Engel, J.P. Perdew. Theory of metallic clusters: Asymptotic size dependence of electronic properties // *Phys. Rev. B*. 1991, v. 43, № 2, p. 1331-1337.
17. M.Y. Gureev, A.K. Tagantsev, N. Setter. Head-to-head and tail-to-tail 180° domain walls in an isolated ferroelectric // *Physical Review B - Condensed Matter and Materials Physics*. 2011, v. 83, № 18, 184104.
18. J. Sanchez, F.L. Tabares, D. Tafalla, et al. Impact of lithium-coated walls on plasma performance in the

- TJ-II stellarator // *Journal of Nuclear Materials*. 2009, v. 390-391, № 1, p.852-857.
19. M. Tatsumisago, M. Nagao, A. Hayashi. Recent development of sulfide solid electrolytes and interfacial modification for all-solid-state rechargeable lithium batteries // *Journal of Asian Ceramic Societies*. 2013, №1, p. 17-25.
 20. J.C. Shank, M.B. Tellekamp, E.X. Zhang, et al. Self-healing of proton damage in lithium niobite (LiNbO₃) // *IEEE Transactions on Nuclear Science*. 2015, v. 62, № 2, 07060733, p. 542-547.
 21. J. Duderstadt, G.A. Moses. *Inertial Confinement Fusion*. New York: «John Wiley & Sons Inc», 1984, 360 p.
 22. M.M. Basko, A.J. Kemp, J. Meyer-ter-Vehn. Ignition conditions for magnetized target fusion in cylindrical geometry // *Nucl. Fus.* 2000, v. 40, № 1, p. 59-68.
 23. O.V. Gotchev, P.Y. Chang, J.P. Knauer, et al. Laser-driven magnetic-flux compression in high-energy-density plasmas // *Phys. Rev. Lett.* 2009, v. 103, p. 215004.
 24. D. Nakamura, H. Sawabe, S. Takeyama. Experimental evidence of three-dimensional dynamics of an electromagnetically imploded liner // *Rev. Sci. Instrum.* 2014, v. 85, p. 036102.
 25. V.V. Kuzenov, S.V. Ryzhkov, V.V. Shumaev. Thermodynamic properties of magnetized plasma evaluated by Thomas-Fermi model // *Applied Physics*. 2014, № 3, p. 22-25.
 26. A.F. Nikiforov, V.G. Novikov, V.B. Uvarov. Quantum-Statistical Models of Hot Dense Matter // *Methods for Computation Opacity and Equation of State*. Basel: «Birkhauser Verlag». 2005, 430 p.
 27. Ya.B. Zel'dovich, Yu.P. Raizer. *Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena*. New York: «Dover Publications», 2002, 944 p.
 28. Yu.V. Boyko, Yu.M. Grishin, A.S. Kamrukov, et al. *Thermodynamic and Optical Properties of Ionized Gases at Temperatures to 100 eV*. Boca Raton: «CRC Press», 1991, 206 p.
 29. S. Dyachkov, P. Levashov. Region of validity of the finite-temperature Thomas-Fermi model with respect to quantum and exchange corrections // *Phys. Plasmas*. 2014, v. 21, № 5, p. 052702.
 30. A.E. Borisevich, S.L. Cherkas. Effect of the conductor radius on the electric explosion dynamics: Magneto-hydrodynamic simulation // *Technical Physics*. 2012, v. 57, № 10, p. 1380-1386.

Article received 05.05.2015

ЧИСЛЕННЫЙ ТЕРМОДИНАМИЧЕСКИЙ АНАЛИЗ СПЛАВОВ ДЛЯ ПЛАЗМЕННОЙ ЭЛЕКТРОНИКИ И ПЕРЕДОВЫХ ТЕХНОЛОГИЙ

В.В. Кузенов, С.В. Рыжков, В.В. Шумаев

Термодинамические свойства (давление, удельная внутренняя энергия и энтропия) смеси ионизованных газов получены на основе теории Томаса-Ферми и модели Саха. Расчеты были сделаны для сплава литий-индий (Li + 10%In), который имеет различные применения в плазменных технологиях.

ЧИСЕЛЬНИЙ ТЕРМОДИНАМІЧНИЙ АНАЛІЗ СПЛАВІВ ДЛЯ ПЛАЗМОВОЇ ЕЛЕКТРОНІКИ І ПЕРЕДОВИХ ТЕХНОЛОГІЙ

В.В. Кузенов, С.В. Рыжков, В.В. Шумаев

Термодинамічні властивості (тиск, питома внутрішня енергія і ентропія) суміші іонізованих газів отримані на основі теорії Томаса-Фермі та моделі Саха. Розрахунки були зроблені для сплаву літій-індій (Li+10%In), який має різні застосування в плазмових технологіях.