Thermal conductivity and thermal diffusivity of the melt Bi-Pb-Sn-Cd at high temperatures. computer experiment

N M Barbin¹,², I V Tikina¹, D I Terentyev¹ and S G Alekseev³

¹Ural Institute of the State Fire Service EMERCOM of Russia, Ekaterinburg, Russia
²Ural State Agrarian University, Ekaterinburg, Russia
³Independent Researcher

E-mail: nmbarbin@mail.ru, tandeos@yandex.ru

Abstract. The method of thermodynamic simulation is used to determine the thermal diffusivity and the thermal conductivity of the melt 42 mass.% Bi-40.6 masses.% Pb-10 masses.% Sn-7.4 mass % Cd depending on temperature. It was found that the thermal conductivity and thermal diffusivity of melts Bi-Pb-Sn-Cd, Bi-Pb-Sn, Bi-Pb differ by no more than 15%. The obtained values indicate the prospects of using this melt as a coolant.

1. Introduction

Liquid metals and their alloys are widely used in various fields of science and technology. A liquid metal coolant of the bismuth-lead-tin-cadmium system with a melting point of about 700°C is known [1]. This alloy contains 13-20% lead and is very expensive. In our work it is proposed to consider a melt with a lead content of 40% and at the same time to maintain the same melting point with a deliberately lower cost, which will expand the scope of its application to large single reactor capacities. The physical and chemical properties of this melt have not been found in the literature. In the event of an accident in a nuclear reactor, boiling of the coolant and melting of the fuel is possible. Therefore, it is necessary to study the behavior of bismuth-lead-tin-cadmium coolant at high temperatures [2].

Thermal diffusivity and thermal conductivity are two of the most important parameters of substances and materials, since they describe the processes of heat transfer and the change in temperature in them. Knowledge of the magnitude of thermal conductivity required for engineering calculations.

In this paper, the dependence of the change in thermal conductivity and thermal diffusivity when heated to high temperatures was obtained.

Due to the complexity of conducting experiments at high temperatures and determining the concentration components in the vapor phase, equilibrium with the alloy, in this work we used the method of thermodynamic modeling.

2. Research methods

Thermodynamic modeling consists in thermodynamic analysis of the equilibrium state of the systems as a whole. The use of thermodynamic modeling allows us to qualitatively predict the composition and properties of complex heterogeneous, multi-element, multiphase systems in a wide range of temperatures and pressures, taking into account chemical and phase transformations [4, 5].
In thermodynamic modeling, condensed individual substances accept compounds with a multiple of the atoms forming them. The composition of the condensed phases includes compounds in the solid (crystalline or amorphous) and liquid states. Individual substances that have the same chemical formula, but are in different phases, are considered to be different compound substances. The constituents of the gas phase are molecules, radicals, atoms, ions, and electron gas.

Model a thermodynamic system with the following features:

• isolated system;
• the system is free from the influence of magnetic, electric and gravitational fields;
• the system is closed, i.e. the exchange of matter or the transfer of matter across its boundaries is impossible.

This is necessary to achieve an equilibrium state.

The program that effectively implements the calculations of thermodynamic systems is the program complex TERRA [6]. The program adopted the following assumptions of the mathematical model:

• closed and isolated systems are considered;
• systems in a state of external and internal thermodynamic equilibrium are analyzed;
• the presence of a gas phase in the system is mandatory;
• all gaseous substances are part of the same gas phase;
• surface effects at the interface are not taken into account;
• individual substances that have the same chemical formula, but are in different phases, are considered different components.

The program complex provides the following features:

• extensive thermodynamic parameters of the system: volume \( V \), the internal energy \( U \), entropy \( S \), enthalpy \( I \), energy Gibbs \( G \), the energy of the Helmholtz \( F \);
• intensive thermodynamic parameter: thermodynamic temperature \( T \), pressure \( P \), density, and molar specific thermodynamic quantity;
• the equilibrium condition of the system with the environment is given by any pair of thermodynamic parameters: \( P, V, T, S, I, U \);
• incorporation in the number of components expected equilibrium composition of any of the individual substances by changing the original data;
• determination of the equilibrium phase composition of the system without prior indication of the thermodynamic admissible states.

The calculation of the composition of phases and equilibrium characteristics is carried out using the reference database on the properties of individual substances. Information basis in the database constitute thermodynamic, thermal and thermo-chemical properties of individual substances, systematized at the High temperature Institute of RAS (database and IVTANTERMO) and at the U.S. national Bureau of standards, the information published in reference [7], and also calculated at the Moscow state technical University on molecular calorimetric and spectroscopic data.

Thermodynamic modeling using the TERRA software package has been successfully used in thermophysics [8 - 13].

The melt Bi-Pb-Sn-Cd is represented by a model of an ideal solution of interaction products. The composition of the melt includes condensed: Bi, Pb, Sn, Cd, PbSn, CdSn, SnBi, BiPb, CdBi, BiSn, BiPb, BiPb, PbBi, PbSn, SnBi, SnBi, SnBi, SnBi, SnBi, SnBi, PbBiSn, PbBiSn, PbBiSn, PbBiSn, PbBiSn, PbBiSn, PbBiSn, PbBiSn, PbBiSn, PbBiSn, PbBiSn, PbBiSn, PbBiSn, PbBiSn, PbBiSn, PbBiSn, PbBiSn, PbBiSn [14]. The existence of these intermetallic compounds is confirmed by literary sources [15].

The equilibrium state in the system is set by the parameters \( T \) and \( P \) and the initial content Bi, Pb, Sn, Cd, Ar. Equilibrium concentrations of condensed and gaseous components are products of all possible reactions between Bi, Pb, Sn, Cd and the gas phase when the system reaches a global
extremum and thermodynamic potential. The thermodynamic parameters of the intermetallic compounds are taken from [16].

Saturated vapor over the melt Bi - Pb - Sn - Cd is represented by the model of an ideal gas of interaction products. The vapor contains gaseous Pb, Bi, Cd, Sn, Pb₂, Bi₂, Bi₃, Bi₄, Sn₂, Cd₂, electron gas, as well as ionized pairs of lead and bismuth, cadmium and tin [17, 14]. These vapor dimers, trimers and tetramers of bismuth, cadmium tin and lead actually exist [18].

The method of thermodynamic modeling studied the behavior of the melt Bi - Pb - Sn - Cd when heated to 3000 K in the atmosphere of Ar. The Ar content in the system was 2% by weight, under these conditions, the vapor can be considered saturated.

Thermal conductivity and thermal diffusivity are determined using the TERRA software package. The thermal diffusivity was calculated by the known formula:

\[ a = \frac{\lambda}{C_p \rho} \]

The reliability of the data obtained is confirmed by testing on a well-studied Pb-Bi system [3].

3. Results

The table presents the thermophysical characteristics of the melt system at \( P = 10^5 \) Pa in the atmosphere of Ar.

**Table 1.** Thermodynamic characteristics of the system (mass%) 42.0 Bi + 40.6 Pb + 10.0 Sn + 7.4 Cd at 300–1500 K and \( P = 10^5 \) Pa in the atmosphere of Ar.

| T, K  | 300  | 400  | 500  | 600  | 700  | 800  | 900  | 1000 | 1100 | 1200 | 1300 | 1400 | 1500 |
|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| \( C_p \), kJ/(kg⋅K) | 0.152 | 0.170 | 0.169 | 0.170 | 0.168 | 0.170 | 0.171 | 0.173 | 0.173 | 0.177 | 0.179 | 0.181 |
| \( \rho \), kg/m³ | 9720  | 9610  | 9480  | 9260  | 9140  | 9020  | 8900  | 8770  | 8650  | 8510  | 8390  | 8270  | 8140  |

Figures 1 and 2 show the changes in thermal conductivity and thermal diffusivity for different pressures in Ar atmosphere.

**Figure 1.** The dependence of the thermal diffusivity of the melt on the temperature in the Ar atmosphere at \( P = 105 \) Pa.
Figure 2. Change in thermal conductivity melt temperature in Ar atmosphere at P = 105 Pa.

Conclusion
The discrepancy between the obtained results and the values presented in the Handbook of thermophysical properties of materials [1] does not exceed 10-15% for heat carriers of similar composition: Bi-Pb, Bi-Pb-Sn and Bi-Pb-Sn-Cd. It can be concluded that the prospects of using this melt as a coolant.

References
[1] Chirkin S V 1968 Thermophysical properties of nuclear engineering materials. Handbook (M.: Atomizdat) p 485
[2] Kashcheev M V, Kuznetsov IA 2007 Sh. tr. m ezhved. Sem. “Heat and mass transfer and properties of liquid metals” 162
[3] Barbin N M, Tikina I V, Terentyev D I, Alekseev S G, Porhachev M Yu 2017 TVT 55 (4) 518–22
[4] Vatolin N A, Moisev G K, Trusov B G 1994 Thermodynamic modeling in high-temperature inorganic systems (M.: Metallurgy) p 352
[5] Moiseev G K, Vyatkin G P, Barbin N M 2002 The use of thermodynamic modeling to study the interaction taking into account ionic melts (Chelyabinsk: Publishing house of SUSU) p 166
[6] Belov G V, Trusov B G 2013 Thermodynamic modeling of chemically reacting systems (M.: MSTU. N. E. Bauman) p 96
[7] Alemasov V E, Dregalin A F, Tishin A P 1971 Thermodynamic and thermophysical properties of combustion products. Ref. in 5 t. (M.: VINITI)
[8] Barbin N M 2008 Chem. physics and mesoscopy 10 (3) 354
[9] Moiseev G K 2006 TVT 44 (2) 311
[10] Engelsht V S, Balan R K 2011 TVT 49 (5) 763
[11] Engelsht V S, Murataliyeva V Zh 2013 TVT 51 (5) 717
[12] Engelsht V S, Murataliyeva V Zh 2013 TVT 51 (6) 848
[13] Barbin N M, Terentiev D I, Alekseev S G 2011 J. Eng. Thermophys. 20 (3) 308
[14] Terentyev D I, Barbin N M, Borisenko A V, Alekseev S G 2012 Prikl. physics. 3 32
[15] State diagrams of double metallic systems T. 1 2001 ed. Lyakishev H I (M.: Mechanical Engineering)
[16] Ovchinnikova I V, Terentyev D I, Alekseev S G, Barbin N M 2011 Melts 5 83
[17] Terentiev D S, Barbin N M, Borisenko A V, Alekseev S G, Popel P S 2011 Chem. physics and mesoscopy 13 (3) 350
[18] Gurvich L V, Weitz I V, Medvedev V L 1982 Thermodynamic properties of individual substances. Ref. and zd. in 4 t. (M.: Science)