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Thermodynamic Calculation of the Phase Diagram for the Al–B–C System at Pressure 7.7 GPa

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Abstract—The phase diagram of the Al–B–C system has been calculated at pressure 7.7 GPa using models of the phenomenological thermodynamics with the interaction parameters derived from the experimental data on the phase equilibria at high pressures and temperatures.

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Keywords: phase diagram, high pressure, high-hardness composites.

A considerable amount of high-hardness industrial ceramics with required functional properties are produced by sintering of powders of substances with covalent types of bonds: diamond, cubic boron nitride, aluminum and silicon nitrides. Compounds of the Al–B–C system belong to this group of substances and offer considerable possibilities to produce high-temperature high-hardness materials. The application of high pressures makes it possible to improve physico-mechanical properties of these materials.

The experimental study of the phase equilibria in the Al–B–C system is reported in [1] and the thermodynamic calculation is made in [2]. The results of the investigations into the phase formation in the Al–B–C system at pressures to 6 GPa are described in [3, 4]. The phase diagrams of the Al–B, Al–C, and B–C binary systems at 8 GPa were calculated in [5–7]. The phase diagram of the Al–B–C ternary system at high pressures has not been constructed.

In our present studies the thermodynamic calculation of the phase diagram of the Al–B–C system is made at pressure 7.7 GPa with the use of the Thermo-Calc software [8] and models of the phenomenological thermodynamics with the interaction parameters derived from the experimental data on the phase equilibria at high pressures and temperatures. The models of phases and the parameters of stability and interaction between the system phases at the ambient pressure were taken from [2]. For the calculations of the phase equilibria in Al–B, Al–C, and B–C binary systems at high pressure the results reported in [5–7] are used. The liquid phase is described in the approximation of subregular solutions, the mixing volume of the ternary system is taken equal to zero. To describe the thermodynamic potential of solid phases the compounds energy formalism (CEF) was used [9]. The baric dependences of molar volumes of the phases are represented by the Murnaghan approximation [10]. The molar volumes of ternary phases under standard conditions $V_{Al_3B_{48}C_2} = 240.7 \times 10^{-6}$ m^3/mole, $V_{Al_{2.1}B_{51}C_8} = 277 \times 10^{-6}$ m^3/mole, $V_{AlB_{40}C_4} = 201.2 \times 10^{-6}$ m^3/mole, $V_{Al_8B_4C_7} = 145 \times 10^{-6}$ m^3/mole are taken from the PDF-2 base [11]. Because of the absence of the data on the compression moduli, their derivatives, and coefficients of thermal expansion for the ternary phases in the literature, the values for AlB_{12} are used [5].

The calculation results are given in Figs. 1–4.

The analysis of isothermal and polythermal cross-sections of the phase diagram of the Al–B–C system at 7.7 GPa shows that the sintering of diamond with aluminum borides will be accompanied by the crystallization of Al_4C_3 carbide from the liquid phase. In the case of the diamond sintering with AlB_2 the amount of the formed Al_4C_3 will be considerable. Since the Al_4C_3 carbide is hygroscopic, it is difficult to expect a long-term life of sintered composites if they are stored in air. At the same time in the Al–B_4C section at the boron concentration above 50 at % there is no equilibrium of the liquid phase with aluminum carbide, which makes possible the production of stable composites during the infiltration of boron carbide powders with liquid aluminum.

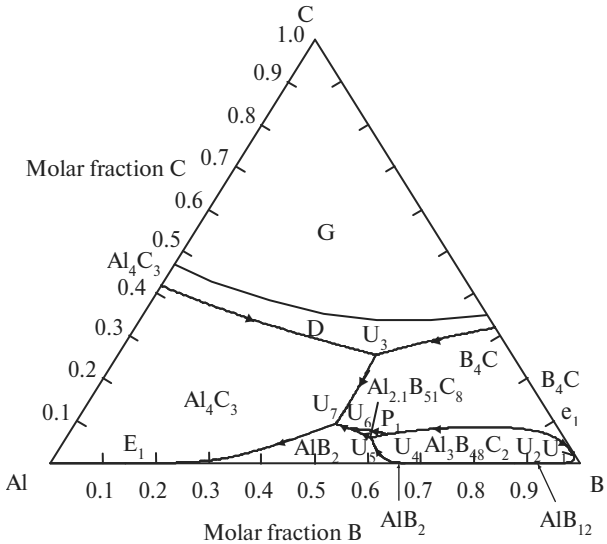

Fig. 1. Projection of the liquidus surface of the phase diagram of the Al–B–C system at 7.7 GPa: G indicates graphite and D—diamond.

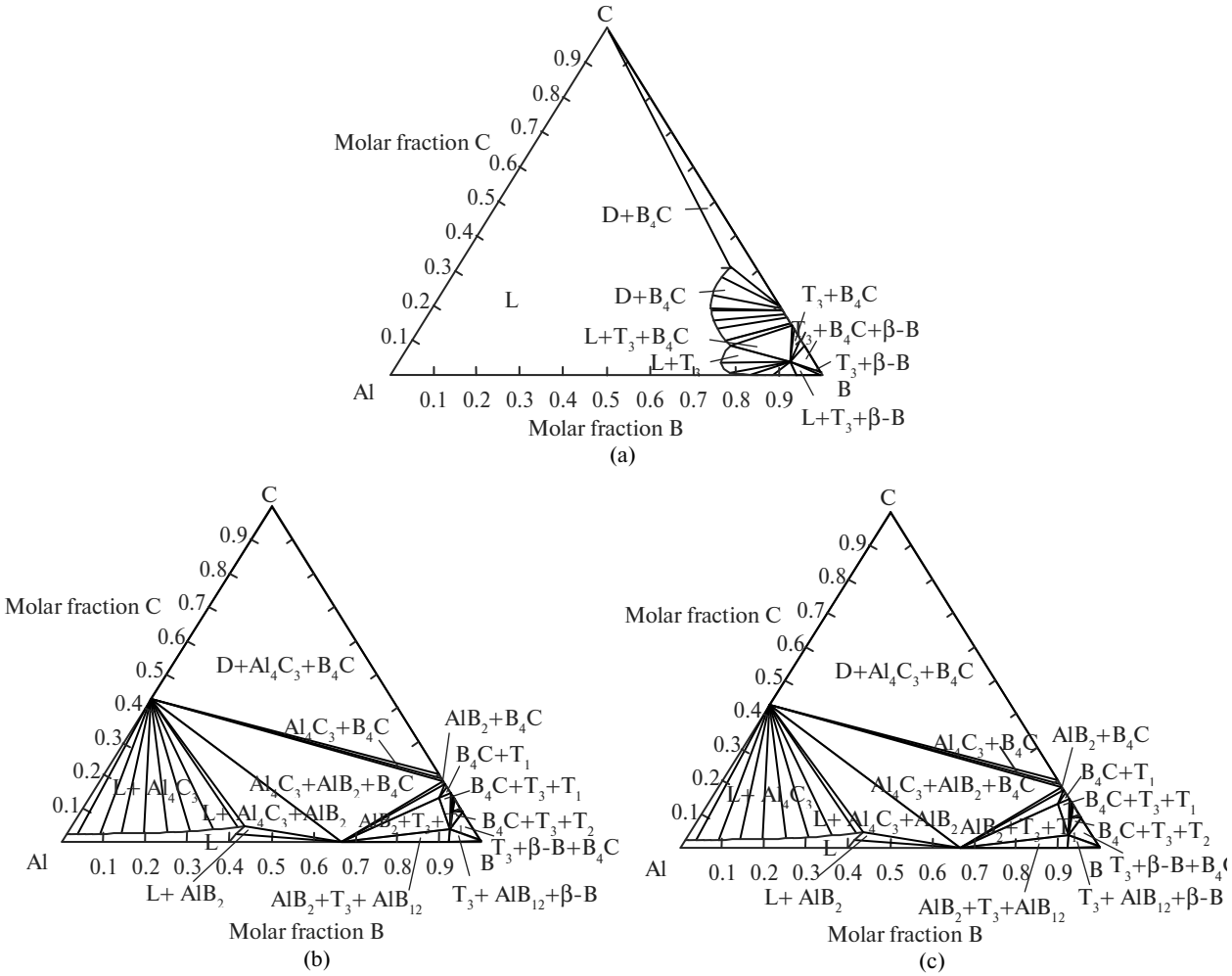

Fig. 2. Isothermal cross-sections of the phase diagram of the Al–B–C system at 7.7 GPa and temperatures 2400 (a), 2100 (b), 1800 (c) K: T_1—$Al_{2.1}B_{51}C_8$; T_2—$AlB_{40}C_4$; T_3—$Al_3B_{48}C_2$; L is liquid; G is graphite; D is diamond.

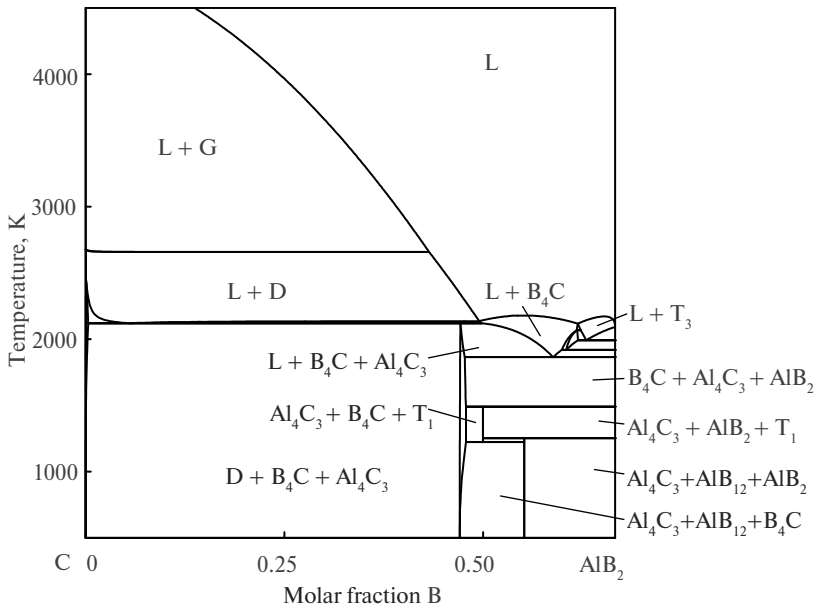

Fig. 3. Polythermal cross-section of the C–AlB_2 phase diagram of the Al–B–C system at 7.7 GPa: T_1—$Al_{2.1}B_{51}C_8$; T_3—$Al_3B_{48}C_2$; L is liquid, G is graphite, D is diamond.

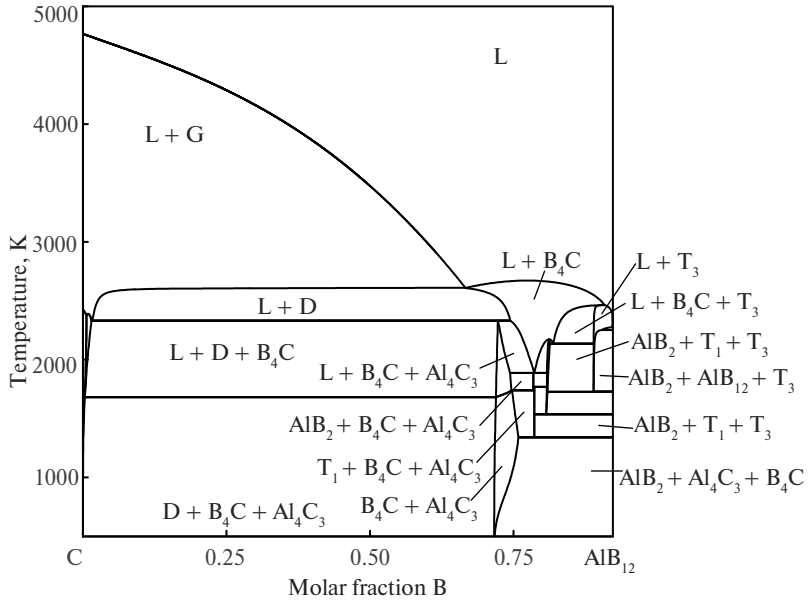

Fig. 4. Polythermal cross-section of the C–AlB_2 phase diagram of the Al–B–C system at 7.7 GPa: T_1—$Al_{2.1}B_{51}C_8$; T_3—$Al_3B_{48}C_2$; L is liquid, G is graphite, D is diamond.

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