INFORMATION, CHRONICLES

INFORMATION ON THE ANNUAL REPORT
OF THE UKRAINIAN COMMISSION
OF PHASE DIAGRAMS AND THERMODYNAMICS (2021)

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The main tasks of the international scientific organization Alloy Phase Diagram International Commission (APDIC), which unites 18 member organizations involving 26 countries, are the exchange of information and coordination of the activities of the international scientific community, mainly in the field of phase diagrams and thermodynamics. The Ukrainian Phase Diagrams and Thermodynamics Commission has been a member of APDIC since 1994. The annual report of the Ukrainian Commission on the results of the activities of Ukrainian scientists in this field in 2020 was presented at the APDIC meeting on June 18, 2021, which was held online due to the coronavirus pandemic. This information is presented in a table, collecting data on the studied systems and obtained result and containing a list of references to published papers. Scientists from the Frantsevich Institute for Problems of Materials Science (National Academy of Sciences of Ukraine, Kyiv), Taras Shevchenko National University of Kyiv (Ministry of Education and Science of Ukraine, Kyiv), and Donbas State Engineering Academy (Ministry of Education and Science of Ukraine, Kramatorsk) provided relevant information to the Ukrainian Commission.

Keywords: APDIC, phase diagram, thermodynamics of phases, annual report.

INTRODUCTION

The Alloy Phase Diagram International Commission (APDIC) was founded in 1986 in Orlando, Florida. Its primary missions include exchanging information and coordinating activities of the international scientific community, mainly in phase diagrams and thermodynamics of phases. The APDIC’s efforts aim to efficiently disseminate data on phase equilibrium and thermodynamics of phases according to the required quality standards. The Commission is interested in many other subjects, including crystallography of intermetallic phases, thermodynamics and kinetics of phase transformations, as well as the combination of basic experimental and theoretical research to promote engineering application of the materials. The members of the Commission independently carry out their individual scientific programmes and meet at annual meetings to discuss urgent matters of coordination of their activities. The APDIC is a nonprofit organization funded through membership fees. Its membership includes 18 organizations representing 26 countries.

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Currently, APDIC is chaired by Dr. Ursula Kuttner (National Institute of Standards and Technology, NIST, Gaithersburg, Maryland, USA).

The Ukrainian Commission on Phase Diagrams and Thermodynamics has been a member of APDIC since 1994. Since creating the Ukrainian Commission over 20 years ago, it has been chaired by Professor Tamara Velikanova (Kyiv, Frantsevich Institute for Problems of Materials Science of the National Academy of Sciences of Ukraine – IPM NASU). Her contribution to the Commission activity and advancing achievements of Ukrainian experts in the field of phase diagrams and thermodynamics within the global scientific community is of great importance. Currently, the Commission’s chairman is Professor Mikhail Turchanin (Kramatorsk, Donbas State Engineering Academy), and the Commission’s secretary is Senior researcher Konstantin Kornienko (Kyiv, IPM NASU).

Following the overall APDIC’s mission, the Ukrainian Commission on Phase Diagrams and Thermodynamics sees the main objective of its work as consolidating the knowledge of chemists, physicists, and materials scientists engaged in physicochemical analysis, alloy thermodynamics, and development of new materials by arranging meetings, schools, and workshops. Membership in APDIC has created new opportunities for professionals to interact directly with their scientific colleagues to obtain up-to-date information on global research, develop joint projects, and prevent inefficient duplication of efforts. The members of the Ukrainian Commission represent departments, chairs, and laboratoires of universities and academic institutions involved in the phase diagrams and thermodynamics in Kyiv, Dnipro, Lviv, Lutsk, Chernivtsi, Uzhhorod, and Kramatorsk.

RESULTS OF ACTIVITIES IN 2020

One of the forms of international cooperation of the Ukrainian Commission is attendance at the annual meeting of the APDIC for information exchange and coordination. APDIC meetings have been held online in the last two years due to the coronavirus pandemic. The 2020 findings of Ukrainian scientists in the relevant industry were presented on 18 June 2021 during the meeting organized by APDIC Secretary Professor Tim Chart (UK) as part of the annual report of the Ukrainian Commission on Phase Diagrams and Thermodynamics. The information was provided to the National Commission by scientists from the Institute of Physics of the National Academy of Sciences of Ukraine, Taras Shevchenko National University of Kyiv (Kyiv National University), and Donbas State Mechanical Engineering Academy (Kramatorsk). A brief summary of the research outcomes is presented in the table below.

At the Frantsevich Institute for Problems of Materials Science, research projects related to studying phase diagrams, phase composition of alloys, and thermodynamics of phases were conducted in the Department of Physical Chemistry of Inorganic Materials, Department of Physical Chemistry and Refractory Oxide Technology, and Department of Functional Ceramics based on Rare Earths. The Department of Physical Chemistry of Inorganic Materials focused on the phase equilibria in ternary systems formed by aluminum with $d$-metals of groups IV–VIII. In particular, a phase diagram of the Al–Co–Cr system was constructed in the region of aluminum content up to 70 at.% based on own experimental data [1]. The phase composition, structure, and properties of TiAl-based alloys doped with 2 at.% Mo were studied [2]. The nature of phase equilibria on the solidus surface of the ternary system formed by a group IV $p$-element (tin) and $d$-metals (cobalt and zirconium) was established using experimental data [3] and the crystal structure of the ternary phase at the Ni–Ti$_5$Sn$_3$ section of the Ni–Sn–Ti system was investigated [4]. Phase equilibria in a system containing refractory borides have been studied, namely the solidus surface of the partial ternary B–Fe–Mo system in the region of boron content of up to 41 at.% was constructed [5]. Consideration was also given to phase composition and properties of some high-entropy alloys of the ternary Mo–Nb–Ti system [6, 7] and other multicomponent systems [8, 9]. Partial and integral mixing enthalpies of the Ba–Sn [10] and Sb–Sr [11] binary systems and Ag–Al–Yb ternary system [12] were determined by isoperibolic calorimetry.

The Department of Physical Chemistry and Refractory Oxide Technology focused on the structure, phase composition, and physical and chemical properties of nanopowders in high-temperature oxide systems. Those included oxides of aluminum, zirconium, and rare earth metals Ce–O–Y–Zr [13] and Al–Ce–Co–O–Y–Zr [14].
| System                      | Reference | Results                                                                                                                                 |
|-----------------------------|-----------|-----------------------------------------------------------------------------------------------------------------------------------------|
| Ag–Al–Yb                    | [12]      | Mixing enthalpies of melts along $x_{Ag}/x_{Al} = 0.46/0.54$ sections at $1271 \pm 1$ K and $x_{Ag}/x_{Al} = 0.19/0.81$ sections at $1454 \pm 5$ K at $x_{Yb} = 0–0.2$ |
| Al–C–Cr                     | [55]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties                                               |
| Al–Ca–O–Si                  | [18]      | Crystal structure of ternary compounds in the CaO–Al$_2$O$_3$–SiO$_2$ system                                                             |
| Al–Ce–Co–O–Y–Zr             | [14]      | Physical and chemical properties of ultrafine powders in the ZrO$_2$–Y$_2$O$_3$–CeO$_2$–Al$_2$O$_3$–CoO system                         |
| Al–Co–Cr                    | [1]       | Phase diagram of the system (solidus and liquidus surfaces, melting diagram, polythermal sections, alloy crystallization scheme at $x_{Al} = 0–0.70$) |
| Al–Co–Cr–Cu–Fe–Ni           | [9]       | Phase composition of six-component high-entropy alloy and features of its strengthening                                                  |
| Al–Co–Cr–Fe–Ni              | [9]       | Phase composition of six-component high-entropy alloy and features of its strengthening                                                  |
| Al–Fe–Ge                    | [19]      | Short-range ordering of melts                                                                                                          |
| Al–Fe–U                     | [24]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties                                               |
| Al–Mo–Ti                    | [2]       | Structure and properties of TiAl-based alloys doped with 2 at.% Mo                                                                       |
| Al–Mo–U                     | [25]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties                                               |
| Al–O–Pu                     | [26]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties                                               |
| Al–Si–U                     | [27]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties                                               |
| B–Fe–Mo                     | [5]       | The solidus surface of the system at $x_B = 0–0.41$                                                                                     |
| Ba–Sn                       | [10]      | Mixing enthalpies of melts for the entire concentration range at $1300$ K, calculation of the liquidus curve                            |
| C–Mo–U                      | [28]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties                                               |
| C–N–U                       | [29]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties                                               |
| Ag–Al–Yb                    | [12]      | Mixing enthalpies of melts along $x_{Ag}/x_{Al} = 0.46/0.54$ section at $1271 \pm 1$ K and $x_{Ag}/x_{Al} = 0.19/0.81$ section at $1454 \pm 5$ K at $x_{Yb} = 0–0.2$ |
| Al–C–Cr                     | [1]       | Phase diagram of the system (solidus and liquidus surfaces, melting diagram, polythermal sections, alloy crystallization scheme at $x_{Al} = 0–0.70$) |
| Al–Co–Cr–Cu–Fe–Ni           | [9]       | Phase composition of six-component high-entropy alloy and features of its strengthening                                                  |
| Al–Co–Cr–Fe–Ni              | [9]       | Phase composition of five-component high-entropy alloy and features of its strengthening                                                  |
| Al–Fe–Ge                    | [19]      | Short-range ordering of melts                                                                                                          |
| Al–Fe–U                     | [24]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties                                               |
| Al–Mo–Ti                    | [2]       | Structure and properties of TiAl-based alloys doped with 2 at.% Mo                                                                       |
| System          | Reference | Results                                                                 |
|-----------------|-----------|-------------------------------------------------------------------------|
| Al–Mo–U         | [25]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Al–O–Pu         | [26]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Al–Si–U         | [27]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| B–Fe–Mo         | [5]       | The solidus surface of the system at $x_B = 0.41$                        |
| Ba–Sn           | [10]      | Mixing enthalpies of melts for the entire concentration range at 1300 K, calculation of the liquidus curve |
| C–Mo–U          | [28]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| C–N–U           | [29]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| C–O–U           | [30]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| C–Pu–U          | [31]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| C–Pu–Zr         | [32]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| C–Rh–Th         | [33]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| C–Rh–U          | [34]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| C–Ru–Th         | [35]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| C–Ru–U          | [36]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| C–Th–U          | [37]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Ce–Mg–O         | [38]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Ce–O–Y–Zr       | [13]      | Structure and phase composition of 90ZrO$_2$–2Y$_2$O$_3$–8CeO$_2$ nanopowder (mol.%) |
| Ce–O–Yb–Zr      | [15]      | Isothermal section of the ZrO$_2$–CeO$_2$–Yb$_2$O$_3$ system at 1100°C |
| Co–Cr–Cu–Fe–Mn–Ni | [8] | Phase composition of six-component high-entropy alloy and features of its strengthening |
| Co–Sn–Zr        | [3]       | The solidus surface of the system                                      |
| Co–Zr           | [21]      | System phase diagram based on the results of thermodynamic optimization |
| Cs–Fe–O         | [39]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Cs–Mo–O         | [40]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Cs–O–U          | [41]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Cs–O–Zr         | [42]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Cu–Hf–Ni–Ti     | [20]      | Thermodynamic properties of liquid alloys using Aassociate Solution Model and forecast of concentration region of their amorphization |
The Department of Functional Ceramics Based on Rare Earths performed fundamental research of phase equilibria in systems with most refractory oxides (with melting temperature above 2000°C), namely, Ce–O–Yb–Zr [15], Gd–La–O–Zr [16], and La–O–Sm–Zr [17].

In the Department of Physical Chemistry at the Taras Shevchenko National University of Kyiv the X-ray diffraction studies on the crystal structure of compounds in the ternary CaO–Al₂O₃–SiO₂ system in liquid and solid states were conducted [18]. The effect of composition on short-range ordering in the melts of the Al–Fe–Ge system was analyzed in wide concentration intervals [19].

In the Laboratory of Physico-Chemical Properties of Metallic Liquid Alloys at Donbas State Mechanical Engineering Academy, the mixing enthalpies of liquid alloys in the Hf–Ni–Ti system were studied for the first time employing high-temperature calorimetry [20]. Temperature–concentration dependence of thermodynamic mixing functions of melts in the Cu–Hf–Ni, Cu–Hf–Ti, Cu–Ni–Ti, Hf–Ni–Ti, and Cu–Hf–Ni–Ti systems has been described in the frameworks of the phenomenological Associate Solution Model. The parameters of the chemical

| System          | Reference | Results                                                                 |
|-----------------|-----------|-------------------------------------------------------------------------|
| Fe–Na–O         | [43]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Fe–O–Pb         | [44]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Fe–U–Zr         | [45]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Gd–La–O–Zr      | [16]      | Isothermal section of the ZrO₂–La₂O₃–Gd₂O₃ phase diagram at 1100°C     |
| Hf–Ni–Ti        | [21]      | Mixing enthalpies of melts along \( x_{\text{Hf}}/x_{\text{Ni}} = 3 \) section at \( x_{\text{Ti}} = 0–0.64 \) and \( x_{\text{Ni}}/x_{\text{Ti}} = 3 \) section at \( x_{\text{Hf}} = 0–0.57 \) at 1873 K; forecast of concentration region of their amorphization |
| La–O–Sm–Zr      | [17]      | Isothermal section of the ZrO₂–La₂O₃–Sm₂O₃ phase diagram at 1100°C     |
| Mg–Ni–Si        | [22]      | Phase diagram of the system (liquidus surface, isothermal cross-sections, alloy crystallization scheme) upon results of thermodynamic optimization |
| Mo–Nb–Ti        | [6, 7]    | Structure, physical and mechanical properties of alloys                 |
| Mo–O–U          | [46]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Mo–Si–U         | [47]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| N–Pu–Zr         | [48]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Ni–Sn–Ti        | [4]       | Crystal structure of the ternary phase on the Ni–Ti,Sn, section         |
| O–Th–Zr         | [49]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| O–U–Zr          | [50]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Pu–Th–U         | [51]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Pu–U–Zr         | [52]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Ru–Si–U         | [53]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |
| Sb–Sr           | [11]      | Mixing enthalpies of melts at 1230 K                                     |
| Th–U–Zr         | [54]      | Critical evaluation of literature data on phase equilibria and thermodynamic properties |

The mixing enthalpies of melts of the Si–Fe–Ge system was analyzed in wide concentration intervals [19]. Temperature–concentration dependence of thermodynamic mixing functions of melts in the Cu–Hf–Ni, Cu–Hf–Ti, Cu–Ni–Ti, Hf–Ni–Ti, and Cu–Hf–Ni–Ti systems has been described in the frameworks of the phenomenological Associate Solution Model. The parameters of the chemical
short-range order in the melts of these amorphous systems were determined as result of the calculations and the concentration regions of their amorphization by melt quenching were forecasted. New thermodynamic descriptions of the Co–Zr [21] and Mg–Ni–Si [22] systems have been developed using the CALPHAD method.

Ukrainian scientists have always displayed great cooperation with a long-standing partner of Materials Science International Services GmbH (MSI) (Stuttgart, Germany). Together, we have prepared the nineteenth issue of the Ternary Alloys handbook, “Selected Systems for Nuclear Applications,” published in December 2019 by MSI [23]. The issue was devoted to the memory of Dr. Gunther Effenberg, who founded and chaired MSI for thirty years, was actively involved in APDIC activities, and cooperated with the Ukrainian Commission. Candidates of Chemical Sciences Dovbenko Oleksandr Ivanovych (IPM NASU) and Dreval Lia Oleksandrivna (DSMA), in collaboration with MSI Publishing House, were engaged in the handbook preparation as associate editors and authors of reviews (together with K.Ye. Korniyenko). In general, critical reviews for 31 systems have been published in this handbook issue. These are Al–Fe–U [24], Al–Mo–U [25], Al–O–Pu [26], Al–Si–U [27], C–Mo–U [28], C–N–U [29], C–O–U [30], C–Pu–U [31], C–Pu–Zr [32], C–Rh–Th [33], C–Rh–U [34], C–Ru–Th [35], C–Ru–U [36], C–Th–U [37], Ce–Mg–O [38], Cs–Fe–O [39], Cs–Mo–O [40], Cs–O–U [41], Cs–O–Zr [42], Fe–Na–O [43], Fe–O–Pb [44], Fe–U–Zr [45], Mo–O–U [46], Mo–Si–U [47], N–Pu–Zr [48], O–Th–Zr [49], O–U–Zr [50], Pu–Th–U [51], Pu–U–Zr [52], Ru–Si–U [53], and Th–U–Zr [54]. Based on the results of participating in the MSI Critical Evaluation Program (Ternary Evaluation Program), a review of Al–C–Cr has been performed [55].

The APDIC will hold its next meeting on 2 July 2022 in Sweden.

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