# Report to APDIC, May 2024



## Associated Phase Diagram and Thermodynamics Committee (APDTC) (Poland, Bosnia&Herzegovina, Bulgaria, Croatia, Czech

Republic, Hungary, Montenegro, Romania, Serbia, Slovakia, Slovenia)

Compiled by: Przemyslaw Fima Ales Kroupa

Presented by: Ales Kroupa

### **Associated Committee**

### <u>SUMMARY</u>

- Associated Committee consists of approx.
  80 members from 10 countries and 28 scientific centers.
- More than 70 scientific studies have been prepared by AC-members and published in 2023 as result of their work, mostly in JCR-indexed journals.

Associated Phase Diagram and Thermodynamics Committee (APDTC)



- 3. The AC-members from Czech Republic, Slovenia, Slovakia, Poland and Romania participated in 14 different domestic and international projects.
- 4. 12 persons worked on their PhD thesis under the supervision of Associated Committee members in 2022.
- 5. Six journals related with thermodynamics and phase equilibria are published in AC-countries.

#### APDTC-members are currently working and/or interested in following topics

Systems	Leading team	Comment
The ternary and multicomponent eutectic alloys of Al, Cu, Mg, Si, and Zn.	University of Belgrade, Technical Faculty, Bor (Serbia)	Good candidates to compete with salts as high- temperature phase change materials in latent heat thermal energy storage applications because of their high volumetric heat of fusion and excellent thermal reliability.
Low melting eutectic alloys based on Ga, Bi and In	University of Belgrade, Technical Faculty, Bor (Serbia)	Low melting eutectic alloys with melting point below 100 °C are showing increasing potentials in various thermal and energy management fields.
Electrical contact materials based on Ag pseudo alloys (composites) dispersion hardened with metal or metal oxide nanoparticles e.g. W, Ni, CdO, SnO2, ZnO, In2O3.	University of Belgrade, Technical Faculty, Bor (Serbia)	Contacts operate under very complex conditions and endure joint and mutually dependent effects of electrical, thermal and mechanical nature. This is reflected in the fact that the heat is generated in a contact pair as a consequence of contact resistance (Joule heating) even under nominal load. This becomes even more evident in nonstandard operating conditions that can potentially generate quite a lot of heat e.g. overload or short circuit load and/or arc formation during make and break operations (pre-close and bounce arcs). Therefore, assessment, simulation, and prediction of electrical contacts' performance under different operating conditions require reliable and accurate thermodynamic parameters and other relevant property data.
Binary and ternary systems with Iridium	Institute of Materials Research, SAS, Kosice (Slovakia)	Subsystems of potentially suitable construction materials for the space industry.

Systems	Leading team	Comment
Wrought aluminium alloys	University of Ljubljana, Department of Materials and Metallurgy (Slovenia)	Thermodynamic and phase diagram calculations are used to predict and optimize various heat treatments for all wrought aluminium alloys. This allows for tailoring the final properties of the material for specific applications.
Casting aluminium alloys	University of Ljubljana, Department of Materials and Metallurgy (Slovenia)	Simulations explore the impact of small changes in alloying elements on cast aluminium alloys. This facilitates the development of new alloys with desired properties and the improvement of existing ones.
Steels	University of Ljubljana, Department of Materials and Metallurgy (Slovenia)	Simulations are employed to understand the influence of different alloying elements and atmospheres on high- temperature oxidation and oxide layer formation in various tool steels. This knowledge improves the design of steels with superior oxidation resistance for specific applications. In addition, simulations were used to model the steel production process itself, enabling optimisation and increased efficiency.
Reaction kinetics	University of Ljubljana, Department of Materials and Metallurgy (Slovenia)	Simulations delve into the formation kinetics of the interaction layer between molten aluminium and tool steels. Additionally, these simulations calculate the thermodynamic stability of carbides within the steel's microstructure and predict the influence of alloying elements on aluminium activity within the steel's matrix. This knowledge is crucial for optimizing the interaction between these materials during processes like casting.

Systems	Leading team	Comment
cemented carbides, heat conductivity, microwave assisted plasma,	University of Miskolc, Miskolc (Hungary)	
nano-materials,		synthesis, CO2 capture, interfacial energy, coherent – strained interfaces, vertically aligned carbon nanotubes,
slags viscosity, wetting transition on steel, electrochemical diagrams,		
molar volume, nucleation, parallel tangent method, phase rule, ESTPHAD (an alternative of Calphad)		Development of theoretical approaches in thermodynamics
crystallization of alloys in space and in magnetic field.		
Binary and ternary systems with Iridium	Institute of Materials Research, SAS, Kosice (Slovakia)	Subsystems of potentially suitable construction materials for the space industry

Systems	Leading team	Comment
Al-Ti-Si-N system	Slovak University of Technology, Faculty of Materials Science and Technology, Trnava	AlTiSiN/TiSiN coatings with TiSiN adhesive layer were investigated. The influence of isothermal annealing on the microstructure and oxidation behavior of nanocomposite coatings was studied. During machining, substantial heat is generated at the interaction area of the cutting tool and the workpiece. Therefore, it is essential to study the oxidation behavior at elevated temperatures to avoid an early degradation of the too
Lead-free solders Sn-Ag-Cu-X (X = Bi, Ga, Ni)	Slovak University of Technology, Faculty of Materials Science and Technology, Trnava	Solder systems Sn-Ag-Cu-X (X = Bi, Ga, Ni) are interesting to study due to the additional elements (Bi, Ga, Ni) which are promising to improve the solders properties. These systems are also suitable for phase-field modeling
Al-Pd-Co system	Slovak University of Technology, Faculty of Materials Science and Technology, Trnava	The aims was to propose an original experimental partial isothermal section of the Al-Pd-Co phase diagram at 1035 °C based on chemical composition of phases present in twelve Al-Pd-Co alloys, annealed detailed study of structure and for long time (300 h) at 1035 °C.

Systems	Leading team	Comment
Se-Sn-X (X = Ti, Fe, Co, Ni)	Masaryk University, Brno (Czech Republic)	The goal of the project is to advance our fundamental understanding of crystal arrangement, thermodynamics and magnetism of selected intermetallic phases both in bulk form and containing interfaces.
Thermoelectric materials – Sb and Zn containing half-Heusler alloys	Masaryk University, Brno (Czech Republic)	study of thermal stability, study of phase diagrams
Bimetallic nanoparticles – Ag-based, Ni-based	Masaryk University, Brno (Czech Republic)	study of thermal stability and surface properties, study of phase diagrams
High entropy alloys – FeCrCoNiCu	Masaryk University, Brno (Czech Republic)	experimental study and thermodynamic
Alloy nanoparticles	Masaryk University, Brno (Czech Republic)	catalysis
High entropy alloys	Masaryk University, Brno (Czech Republic)	magnetic properties
Al-based binary and ternary based systems, e.g. Al-Co-Si, Al-Ge-Mg, Al Ge-Sn etc.	Institute of Physics of Materials, CAS, Brno (Czech Republic)	The importance of Al-based system in industrial applications is clear and not all information about phase diagram and properties of phases are known.
Se-Sn-X (X = Ag, Co, Fe, Ni, Pb, Te, Ti	Institute of Physics of Materials, CAS, Brno (Czech Republic)	The goal is to advance our fundamental understanding of complex phase diagrams, crystal arrangement, thermodynamics and magnetism of selected intermetallics, materials are promising as future advanced materials for photovoltaics, superconductors, thermoelectrics, etc.

Systems	Leading team	Comment
Synthesis and complex characterization of ternary alloys La-Ni-M (M=Cu, In, Mg, Sn) over wide temperature range for the use for H storage.	Institute of Physics of Materials, CAS, Brno (Czech Republic)	Hydrogen has a promising perspective as an energy carrier with the potential being clean and efficient energy source in various applications. One type of promising material for this type of energy storage are solid metal hydrides based on suitable elements. The aim of the project is to study properties and perspectives of a new group of hydrides.
Phase stability of CrSBr layered A- type antiferromagnet	University of Chemistry and Technology, Prague, (Czech Republic)	
La-Al-Mg-O system	University of Chemistry and Technology, Prague, (Czech Republic)	hexaaluminates as matrices for optically active dopants (RE3+)
RE-Ba-Cu-O system	University of Chemistry and Technology, Prague, (Czech Republic)	REBCO based high temperature super conductors
Steels	VSB Technical University of Ostrava, (Czech Republic)	lack of knowledge regarding phase diagrams
Ternary La Ni based systems	VSB Technical University of Ostrava, (Czech Republic)	lack of thermodynamic, thermophysical and kinetic data, potential phases for hydrogen storage
Sb-based intermetallic compounds	Institute of Metallurgy and Materials Science, Krakow	Heat capacity, thermal stability.
Systems: Mg-Pb-Pd, Ag-Mg-Pd, Ag- Ti, In-Li, Sb-Te	Institute of Metallurgy and Materials Science, Krakow	Research on energy and hydrogen storage materials.

Systems	Leading team	Comment
Multicomponent metallic systems with gallium	AGH University of Science and Technology, Krakow, (Poland)	as a new functional materials
Heusler alloy, Laves Phase intermetallic compounds and their solid solutions.	Institute of Low Temperature and Structure Research, Wroclaw (Poland)	The studied compounds are characterized by their respective magnetocaloric and magnetic properties. Depending on the properties, they can find application in pro-ecological magnetic refrigeration both at room temperatures and in cryogenics. For example, for the liquefaction of hydrogen.
Ca2Nb2O7–Nd3NbO7, CaO– Nd2O3–Nb2O5	University of Economics and Business, Wroclaw (Poland)	niobates formed in these systems shows perspective luminescent properties
Rare earth MOFs	University of Economics and Business, Wroclaw (Poland)	luminophores and adsorbents (for arsenates and phosphates) for sensing devices in food technology; environment friendly syntheses of MOFs;
Calcium hydroxyapatites from egg shells	University of Economics and Business, Wroclaw (Poland)	low crystalline materials with better bioavailability;
Modified aluminide coatings	Rzeszow University of Technology (Poland)	Modified aluminide coatings are applied in aircraft industry to protect engine blades from hot corrosion.
micro and nanomaterials/functional materials; high entropy materials; nano/bio interfaces	Institute of Physical Chemistry "Ilie Murgulescu" of the Romanian Academy (Romania)	Thermodynamic properties and thermodynamics of processes.

### **Associated Committee in 2023**

Country	Scientific centers	AC- members	Papers published	Grants ongoing	BSc students	MSc & PhI students	Granted MSc & PhI degrees
Bulgaria	4	5	7	0	0	0	0
Croatia	1	1	4	0	0	1	0
Czech Republic	4	16	7	3	11	6	1
Hungary	1	5	7	2	0	1	0
Montenegro	1	1	2	0	0	0	0
Poland	7	24	24	3	0	1	4
Romania	1	3	3	2(1)	0	0	0
Serbia	6	18	5	1	6	4	2
Slovakia	2	7	8	4	0	2	0
Slovenia	1	3	12	2	_*	8	4

\* Not available

### **Associated Committee members**

POLAND					
AGH – University of Science and Technology Faculty of Non-ferrous Metals	Stanislaw Malecki Boguslaw Onderka Dominika Jendrzejczyk- Handzlik	Wroclaw University of Technology Faculty of Chemistry Group of Chemical Metallurgy	Leszek Rycerz Ida Chojnacka Anna Dańczak Marek Jasiorski Szczepan Roszak		
Rzeszow University of Technology	Jolanta Romanowska	Institute of Low Temperature and Structure Research	Jacek Ćwik		
Wroclaw Medical University Department of Analytical Chemistry	Wiesław Gaweł Igor Mucha	Wrocław University of Economics and Business Faculty of Engineering and Economics, Department of Inorganic Chemistry	Aleksandra Pelczarska Beata Salamon Bożena Pilarek		
Institute of Metallurgy and Materials Science, Polish Academy of Sciences	Wladyslaw Gasior Tomasz Czeppe Adam Debski Przemyslaw Fima	Grzegorz Garzel Tomasz Gancarz Piotr Ozga	Anna Wierzbicka–Miernik Anna Sypien		

CROATIA		MONTENEGRO		
University of Zagreb Faculty of Metallurgy - in Sisak	Tamara Holjevac-Grgurić	<b>Montenegro University</b> Faculty of Metallurgy and Chemical Technology	Vanja Asanovic	

### Associated Committee members

BULGARIA				
<b>University of Plovdiv</b> Faculty of Chemistry	Georgi Patronov Georgui Vassilev	Univ. Food Technology - Plovdiv Department of Materials ScienceVanya Gandova		
<b>University of Ruse</b> Department of Materials Science	Parvoletka Docheva	<b>Medical Univ of Plovdiv</b> Faculty of Pharmacy, Dept. Chemical Science	Nikolina Milcheva	
	CZECH	REPUBLIC		
Masaryk University, Brno	Pavel Broz Jana Pavlu Mojmir Šob Jiri Sopousek Jan Vrestal Monika Vsianska	Institute of Physics, AS CR, Brno	Jiri Bursik Tomas Kana Ales Kroupa Milan Svoboda Adéla Zemanová Ondrej Zobac	
Institute of Chemical Technology, Prague	David Sedmidubsky	Technical University of Ostrava, Ostrava	Bedřich Smetana Monika Kawolukova Simona Zla	
HUNGAI	RY	ROMANIA		
University of Miskolc, Miskolc	George Kaptay Andras Roosz Tamas Mende Ádám Végh József Korózs	Institute of Physical Chemistry "I.G. Murgulescu" of the Romanian Academy	Speranta Tanasescu Cornelia Marinescu Florentina Maxim	

### Associated Committee members

SLOVAKI	۹	SLOVENIA		
Faculty of Materials Science and Technology (Trnava), Slovak University of Technology in Bratislava	Roman Čička Marián Drienovský Marián Palcut Jozef Krajčovič Ivonka Černičková Libor Ďuriška	<b>University of Ljubljana,</b> Department of Materials and Metallurgy, Faculty of Natural Sciences and Engineering	Jozef Medved Maja Vončina Tilen Balaško	
Institute of Materials Research, SAS, Kosice	Viera Homolova			
	_SER			
	JLI			
<b>University of Belgrade</b> , Technical Faculty, Bor	Dragan Manasijević Nada Strbac Ljubiša Balanović	Uroš Stamenković Ivana Marković Srba Mladenović	Saša Marjanović Milan Gorgievski	
Mining and Metallurgy Institute, Bor	Ana Kostov Aleksandra Milosavljevic	<b>University of Belgrade,</b> Institute of Chemistry, Technology and Metallurgy Faculty of Technology and Metallurgy, Belgrade	Nadezda Talijan Vladan Cosovic Vaso Manojlović	
Institute for nuclear and other raw materials, Belgrade	Miroslav Sokic Branislav Markovic	<b>University of Pristina,</b> Faculty of Technical Sciences, Kosovska Mitorvica	Dusko Minic Milena Zečević Aleksandar Dordevic	

#### Journals related with thermodynamics and phase equilibria published in AC-countries

Archives of Metallurgy and Materials, IF = 0.6, Citescore = 1.2,https://www.journals.pan.pl/ammOpen Access

Journal of Mining and Metallurgy Sect. B Metallurgy, IF = 1.0, Citescore = 2.1,http://www.jmmab.com/Open Access, no publication fees

**Journal of Thermal Analysis and Calorimetry**, IF = 4.4, Citescore = 9.1, <u>https://www.springer.com/journal/10973</u>

Kovove Materialy – Metallic Materials, IF = 0.7, Citescore = 1.5,http://www.kovmat.sav.sk/Open Access, no publication fees

**Metalurgija**, Citescore = 1.2, https://pubweb.carnet.hr/metalurg/journal-metalurgija-2 Open Access

**Revue Roumaine de Chimie**, IF = 0.5, Citescore = 0.8 https://revroum.lew.ro/



# Conferences related with thermodynamics and phase equilibria organized in APDTC-countries

11th Symposium on Thermodynamics and Phase Diagrams, 23-24 June 2023, Kosovska Mitrovica (Serbia).

54th International October Conference on Mining and Metallurgy, October 18 -21, 2023, Bor, Serbi, <u>https://ioc.tfbor.bg.ac.rs/</u>

63rd IFC Portoroz 2023 = 63. IFC Portorož 2023, 13-15 September 2023, Portoroz, Slovenia

28th International Conference on Materials and Technology : 11–13 October 2023, Portorož, Slovenia

International Conference of Physical Chemistry (ROMPHYSCHEM 17), 25-27 Septembrie 2023, Bucuresti, Romania (S.Tanasescu - Member in the Organizing Committee; F. Maxim – Member of the Conference Secretariat )

Termoanalytical seminar TAS 2023, Brno, co-organized by IPM CAS.

SURFINT-SREN VIII: Progress in Applied Surface, Interface and Thin Film Science - Solar Renewable Energy News VIII, 20-22 November 2023, Hotel SUZA, Bratislava, Slovakia\*

IEEE NAP 2023: IEEE Nanomaterials: Applications and Properties, 10-15 September 2023, Crowne Plaza Hotel, Bratislava, Slovakia\*

(\* Only small part of the conference related to APDIC topics)

#### Selected books and monographs published in APDTC-countries

J. Ćwik, Intermetallic Compound (Volume II) 2023, MDPI, ISBN 978-3-0365-9547-4

Phase equilibria in the subsolidus region of CaO–Nd2O3–Nb2O5 ternary oxide system and physicochemical properties of the phases, dissertation, Bożena Pilarek, Supervisor: prof. dr hab. inż. Irena Szczygieł

S. Kulawik, Thermodynamic properties of liquid Ga-Sn-Zn and Ga-In-Zn alloys, PhD Thesis ISBN: 978-93-60768-73-0

Awards granted in the reported year

G. Kaptay was awarded Szechenyi prize (highest academic prize in Hungary)