Summary of Phase Diagram Activities in the UK

Materials Chemistry Group
Institute of Materials, Minerals and Mining

Summary Report to APDIC, May 2024

The UK member for APDIC is the *Institute of Materials, Minerals and Mining* (IOM3), and is represented at APDIC by the chair of the *Materials Chemistry Group* (MCG), a sub-group of the new Technical Community, *The Materials Characterisation and Properties Group*. The MCG aims to represent the IOM3 membership who have an interest in Materials Chemistry, and of course, phase diagrams, phase equilibria and thermodynamics. As the *Institute of Metals*, the IOM3 was one of the founding members of APDIC, and the representative body was the predecessor at that time was *the Phase Diagram Committee*. In 2018, the IOM3 acquired a new CEO, and this has resulted in a restructuring of the Institute and its technical communities along the lines of 'The Materials Cycle' covering all aspects of 'Materials' from the raw material (extraction), through processing and design, applications to reuse and recycling. As part of this restructuring, the 40+ technical committees, groups and divisions were reduced to 20 technical communities with each run by a *board*. As part of this process, the *Materials Chemistry Committee* (MCC) was dissolved and replaced by a virtual sub-group, the MCG, with the chair (*the Technical Champion*) sitting on the board of the *IOM3 Materials Characterisation and Properties Group* representing those of the membership with an interest in Materials Chemistry.

As a result of the restructuring process and the accompanying consultation period there has been relatively little activity undertaken by the MCG. The IOM3 continues to be the member to APDIC, and the representative is the 'Technical Champion', who at present is Andy Watson, current chair of the MCG. However, membership of the Technical Community boards is for a strictly 4-year term with replacements being selected by interview following advertisement to the whole membership through the Institute magazine, *Materials World*.

The remit of the MCG remains the same as the MCC and the *Phase Diagram Committee* before that. Its main task has been to coordinate critical assessment and experimental work on phase diagrams within the UK and disseminate this information to industry. As part of this dissemination, the *Phase Diagram Committee* authored a number of phase diagram reviews that were published by the Institute. Its remit now, as the MCG, is to represent the members of the IOM3 who have an interest in Materials Chemistry and is therefore more diverse in its activities.

This, report to APDIC will focus on the activities of its members for 2023.

The membership of the MCG aims to be a balance between providers and users of phase diagram and thermodynamic information and in the past has benefited from a

strong industrial input. The committee provides a forum to identify industrial needs, a discussion group between specialists and a focus within the *IOM3* for active national and international collaboration on the provision of assessed data, on modelling, and on theoretical and computational aspects of phase equilibria in materials.

The committee is interested in all aspects of the phase equilibria, including metastable equilibria and kinetics, in all classes of engineering materials and covering both fundamental and applied topics. It recognises the vital role that reliable information on both phase diagrams themselves and on the rates of approach to equilibrium plays in under-pinning many spheres of materials science and technology. The Materials Chemistry Group is concerned not only with metals and alloys but also ceramics, slags, salts, semiconductors, superconductors, glass, nuclear materials and polymers. The committee encourages all aspects of experimental and theoretical work relating to phase equilibria in materials systems ranging from direct studies of phase diagrams and the determination of thermodynamic mixing parameters to the thermodynamic modelling of phases and *ab initio* calculations of phase stability and microstructure.

Meetings

An important aim of the MCG to support and expand the UK Thermodynamics community. This will be achieved in part through meetings and seminars organised under the IOM3. It is proposed to run the *Annual Thermodynamics of Materials Seminar* as in previous years. Planning is already underway for *AToMS2025* with a tentative date and venue set for June 24th-25th at Bangor University in Wales.

A part of effort to enlarge the UK thermodynamics community involves a degree of training. In previous years, the MCC held the successful *Hume-Rothery Seminar*, a two-day demonstration event in association with SGTE (Scientific Group Thermodata Europe), and plans are underway to revive this event with a possible meeting aimed for early 2025.

The MCG itself currently meets monthly and incorporates a scientific discussion element to the meetings.

Interactions with Other APDIC members

APDIC MSI

Andy Watson continues to work with MSI on their evaluation programme and has contributed to recent volumes of the *Ternary Alloys* series. Andy was also heavily involved with the *7th MSIT Winter School on Materials Chemistry* along with Hari Kumar from Indian Institute of Technology, Madras, (APDIC India).

Current Membership of the Materials Chemistry Group of the IOM3

As stated previously, the *MCC* ceased to exist as a technical committee of the *IOM3* during April 2022. The new Group is still growing, and the list of active members is given below. Note that there is now an 'International Membership'. This is made up of those that have, or have had, some association with the group and would like to interact on a more frequent basis by attending the online monthly meetings. They are also current (or previous) members of the IOM3.

		Institution
Wahab	Abdul	University of Sheffield
Marcus	Bannerman	University of Aberdeen
Tim	Chart	Chart associates
Kathy	Christofidou	University of Sheffield
Teresa	Davey	Bangor University
Alan	Dinsdale	Hampton Thermodynamics/
George	Chen	The University of Nottingham
Derek	Fray*	University of Cambridge
John	Gisby	Hampton Thermodynamics
Chris	Gourlay	Imperial College
Duncan	Gregory	University of Glasgow
Theodore	Hanein	University of Leeds
Girish	Kale	University of Leeds
Hajime	Kinoshita	University of Sheffield
Chancel	Mawalala Moundounga	University of Sheffield
Stuart	Mucklejohn	Université de Toulouse
Duncan	Putman	Rolls Royce Plc
Carsten	Schwandt*	University of Cambridge
Andrew	Scott (sec)	University of Leeds
Dimitra	Spathara	University of Birmingham
Howard	Stone	University of Cambridge
Mark	Tyrer	Collegium Basilea
Claire	Utton	University of Sheffield
Nils	Warnken	University of Birmingham
Andy	Watson (chair)	Hampton Thermodynamics
International Members		
Lesley	Cornish	University of Witwatersrand (S. Africa)
Mudith	Karunaratne	Sri Lanka Institute of Information
Begoña	Santillana	Tata Steel (Netherlands)

** Corresponding membership*

Phase Diagram Activities in the UK:

(Please note, this list may not be exhaustive and many of the studies are ongoing, continuing from previous years)

Interest	Material/system	Researcher(s)
	Fe-Ti-Mo,W Al-Fe-V	University of Birmingham (Sandy Knowles, Paraic O'Kelly) and Hampton Thermodynamics (Andy Watson)
High entropy alloys	Cr-Mn-Fe-Co-Ni-Mo-Nb-Al-Ti-C	University of Cambridge (Howard Stone, Rosie Mellor), University of Manchester (Ed Pickering), University of Sheffield (Kathy Christofidou)
800˚C phase equilibria studies, several alloys from the system. Part of larger program aimed at understanding increased additions of Co and Ti to Ni-based superalloys.	Ni-Co-Cr-Fe-Mo-W-Al-Ti-Nb-Ta-Hf-C-B-Zr	University of Cambridge (Howard Stone) & University of Sheffield) Kathy Christofidou)
Cupronickel alloys	Al-Cu-Ni	”
As part of the efforts to understand high entropy alloys. Phase equilibria studies 500-900˚C temperature range.	Fe-Cr-Co-Ni-Mn	University of Cambridge (Howard Stone, Nick Jones & Maximilian Bloomfield) University of Manchester (Ed Pickering), University of Sheffield (Kathy Christofidou)
Phase stability of V-based multi-principal element alloys	V-Cr-Mn-Fe V-Cr-Mn-Fe-Al	University of Manchester (Ed Pickering)
Development and maintenance of COST 531 and MP0602 lead-free solders databases	Ag-Au-Bi-Cu-In-Ni-Pb-Pd-Sb-Sn-Zn + Ga, Ge, Mg, Si	Hampton Thermodynamics (Andy Watson)
Management of general database (SGSOL) on behalf of SGTE		”
MSI evaluation programme - review	Co-Fe-Ho Co-Fe-Nd Cr-Cu-Ti	”… in cooperation with U of Wittwatersrand (Lesley Cornish), CAS Czechia and RTH Aachen University of Birmingham (Dimitra Spathara)
Amalgams for light sources	Ga-In-Hg $GaCl_3$-InCl	Hampton Thermodynamics (Andy Watson) and Université de Toulouse (Stuart Mucklejohn)
Development and maintenance of COST 531 lead-free solders database	Ag-Au-Bi-Cu-In-Ni-Pb-Pd-Sb-Sn-Zn	Hampton Thermodynamics (Alan Dinsdale)
	Li-Mg	”
Management of database for elements on behalf of SGTE		”
Reassessment of data for the elements.	Ag, Be, Bi, Cd, Cs, Cu, Ge, Hg, In, K, Li, Mg, Na, Rb, Sb, Si, Sn, Tc, Zn	”
Al-alloys	Mg-Si	BCAST (Brunel University – Alan Dinsdale)
	Al-Si Si-Zn Al-Si-Zn Al-Ge Ge-Sn Al-Sn Al-Ge-Sn	Hampton Thermodynamics (Alan Dinsdale, with Czech Academy of Sciences and Austrian Research Foundation)
Electronic solders	Sn-Bi; Sn-Cu-Ni	Imperial College (Chris Gourlay & Sergey Belyakov)
Solid electrolytes and cathode materials	Re_2O_3-CeO_2-Gd_2O_3, Re_2O_3-SrO-CoO-	University of Leeds

Interest	Material/system	Researcher(s)
in Solid Oxide Fuel Cells	Fe_2O_3 and Re_2O_3-BaO-CoO-Fe_2O_3	(Girish Kale)
Phase stability by DFT: bulk and multilayer for photonic applications	Thin-layer transition metal dichalcogenides	University of Leeds (Andrew Scott)
High-entropy alloys for next generation nuclear applications.	V-Cr-Mn Ti-V-Cr-Mn Ti-V-Cr-Mn-Fe Ti-V-Ta-W Ti-Ta-W Ti-V-W Ti-V-Ta-W(low)-Fe(low) Ti-V-Ta-W(low)-Cr(low) V-Cr-Mn-Fe-W(low)	University of Manchester (Ed Pickering) Univ. of Sheffield (Amy Gandy) Oxford University (David Armstrong) and partners in India
High-entropy alloys for brazing applications	Cr-Mn-Ni-In B-Cr-Fe-Ni-Ge	University of Manchester (Ed Pickering) Univ. of Sheffield (Russell Goodall)
Materials development and process understanding	Fe-C	Rolls Royce (Duncan Putman)
On-going materials development	Ni-based alloys	”
Modelling hydride formation in zircaloys, as well as oxidation and alloy design in Nb-based alloys	Zircaloys, Nb-based alloys	University of Sheffield (Claire Utton)
Relating to reprocessing of UK nuclear waste	Cs-O-Re Cs-O-Tc	University of Sheffield (Claire Utton/Hajime Kinoshita)
Refractory alloys for aerospace	Nb-Si-Al, B, Ge, Ti	University of Sheffield (Claire Utton/Hajime Kinoshita/Panos Tsakiropoulos)
calcium sulfoaluminate cement clinker	CaO-Al_2O_3-SiO_2-SO_3-Fe_2O_3-$CaCl_2$–MgO-P_2O_5	University of Leeds (Theodore Hanein)
calcium (alumino)ferrites in relation to cement clinker.	CaO-Fe_2O_3-Al_2O_3-MgO-ZnO-TiO_2-Na_2O	University of Leeds (Theodore Hanein)
Modelling of blended cement hydration.	CaO-SiO_2-Fe_2O_3-Al_2O_3-MgO-Na_2O-K_2O	Mark Tyrer (Collegium Basilae) In collaboration with TU Dublin (Niall Holmes) http://www.hydcem.com/
High temperature phase diagram studies in cooperation with ESA	Al-Fe-Si	Begoña Santillana (TATA Steel)
Assessment. Cements	CaO-SiO_2-Al_2O_3-FeO-Fe_2O_3-O_2	University of Aberdeen, (Marcus Bannerman)
MSI evaluation programme – review. Extremely radiopure electroformed/electroplated, strengthened alloys for Dark Matter detectors	Cr-Cu-Ti	University of Birmingham. (Dimitra Spathara)
Modelling. High voltage cathodes for current and next generation Li-ion batteries	Li-Ni-Mn-Co-O	University of Birmingham. (Dimitra Spathara)

Interest	Material/system	Researcher(s)
Assessment. Using machine learning to predict free energies in HEA's	Al-Cr-Cu-Fe-Ni	University of Leeds. (Andrew Scott)
Experimental. Heat contents (ΔHT-298.15K :from 900K to 1200K) and heat capacities (at low T, from 1.8K to 300K)	$Ca_5(SiO_4)2SO_4$ $Ca_{10}(SiO_4)3(SO_4)3Cl_{2-x}F_x$	University of Sheffield. (Chancel Mawalala Moundounga)
Comprehensive database development for oxide systems	Al-C-Ca-Fe-Si C-Cr-Fe-Mn-Mo-Ni-Si Al-C-Ca-Cr-Fe-Si-Ti-V C-Fe-Mn-P Ce-Co-Cu-Fe-Ni-O-S Ag-Ce-Co-Cu-Fe-Ni-Pd-Pt-Rh Ag-Ce-Co-Cu-Fe-Ni-Pd-Pt-Rh-O-S Ag-Au-Ce-Co-Cu-Fe-Ni-Pd-Pt-Rh-O-S As-Bi-Cu-Fe-Ni-Pb-Sb-O-S As-Bi-Cu-Fe-Ni-Pb-Sb-Zn-O-S Al-Ba-Ca-Mg-Mn-O-P-Si Al-Ba-Ca-Co-Cr-Cu-Fe-Mg-Ni-O-Pb-Si-Zn Al-Ca-Fe-Mg-Ni-O-P-Si Al-Ca-Fe-Mg-Na-Ni-O-P-S-Si-V-Zr Al-Ca-Co-Cr-Cu-Fe-Mg-Ni-O-P-Pb-Si-Zn Al-Ca-Co-Cr-Cu-Fe-Mg-Ni-O-P-Pb-Si-Zn-Zr Al-Ca-Ce-Co-Cr-Cu-Fe-Mg-Ni-O-Pb-Si-Zn Al-Ca-Co-Cr-Cu-Fe-La-Mg-Ni-O-Pb-Si-Zn Al-Ca-Co-Cr-Cu-Fe-Mg-Ni-O-Pb-Si-Zn-Zr Al-Ca-Ce-Co-Cr-Cu-Fe-Mg-Ni-O-Pb-Si-Zn-Zr Al-As-Ca-Co-Cr-Cu-Fe-Mg-Ni-O-Pb-Si-Zn Al-Bi-Ca-Co-Cr-Cu-Fe-Mg-Ni-O-Pb-Si-Zn Al-Ca-Co-Cr-Cu-Fe-Mg-Ni-O-Pb-Sb-Si-Zn Al-Ca-Cr-Fe-Mg-Na-O-Si-Ti-Zr Al-Ca-Fe-Mg-Mn-Na-O-Si-Ti-Zr Al-Ca-Fe-K-Mg-Na-O-Si-Ti-Zr Al-Ca-Fe-Mo-Na-Mg-O-S-Si-Zr Al-Ca-Fe-K-Mg-Mo-Na-O-S-Si-Zr Al-Ca-Cl-Fe-K-Mg-Na-O-S-Si Al-Ca-Fe-K-Mg-Na-O-S-Si-Sn Ca-Fe-H-Na-O-S-Sn	Hampton Thermodynamics (John Gisby)