Summary of Phase Diagram Activities in the UK

Materials Chemistry Committee
Institute of Materials, Minerals and Mining

Summary Report to APDIC, May 2011

One of the main tasks of the Materials Chemistry Committee of the Institute of Materials, Minerals and Mining is to coordinate critical assessment and experimental work on phase diagrams within the UK and disseminate this information to industry. The membership of the committee is a balance between providers and users of phase diagram and thermodynamic information and benefits from a strong industrial input. The committee provides a forum to identify industrial needs, a discussion group between specialists and a focus within the Institute of Materials, Minerals and Mining 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 current Chairman of this committee is Dr Andy Watson of the IMR/SPEME, at the University of Leeds.

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 play in under-pinning many spheres of materials science and technology. To this aim it seeks:

- to co-ordinate critical assessments and experimental work in various organisations and institutions in the UK
- to avoid undue overlap of experimental studies
- to encourage and nurture international co-operation on phase diagram knowledge.

The Materials Chemistry committee 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.

The committee also seeks to support academic institutions in their role in the teaching of thermodynamics and phase equilibria and to ensure that materials scientists in industry have adequate training in this area of fundamental importance.

As part of an ongoing initiative, the committee is preparing a *Strategy Document* for Materials Chemistry in the UK. It is felt that the Materials Chemistry community is under serious threat as research funding and teaching are being squeezed. Once completed, the document will be circulated to funding bodies in attempt to address this problem. It will receive official sanction from the IoM3. As part of this initiative, the *Materials Chemistry Committee* will play host to the next *World Round Robin Seminar*, which will take place in 2012. The seminar will be a 'fringe' session at the Institute's *Materials Congress* that will take place in London in June.

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Membership of the Materials Chemistry Committee of the IoM3:

		Institution
Tim	Chart	Chart associates
Alan	Dinsdale	NPL
George	Chen	The University of Nottingham
Derek	Fray*	University of Cambridge
Alan	Gibbon*	MIRO
Eleanor	Jay	Imperial College
Neil	Jones	CORUS
Girish	Kale	University of Leeds
Hudai	Kara*	Oakdene Hollins
Mudith	Karunaratne	University of Loughborough
Hajime	Kinoshita	University of Sheffield
Stuart	Mucklejohn	Nottingham Trent University
Keith	Parker	GE Lighting
Carsten	Schwandt	University of Cambridge
Andrew	Scott (sec)	University of Leeds
Guosheng	Shao	University of Bolton
Derek	Sinclair	University of Sheffield
Rachel	Thomson*	University of Loughborough
Mark	Tyrer	UCL/MIRO
Andy	Watson (chair)	University of Leeds

* *corresponding membership*

Phase Diagram Activities in the UK*:*

(Details are given on the **Report Table** on the *APDIC* website)

Interest	Material/system	Researcher(s)
Development and maintenance of COST 531 lead-free solders database	Ag-Au-Bi-Cu-In-Ni-Pb-Pd-Sb-Sn-Zn	NPL (Alan Dinsdale)
Development of aluminium database for modelling of thermophysical properties associated with solidification	Al-B-Cu-Fe-Mg-Mn-Ni-Ti-Zn	”
Systems associated with high-temperature lead-free solders. HISOLD: COST MP0602	Ag-Al-Au-Ge-Cu-Mg-Ni-P-Pb-Sn-Zn	”
COST535	Fe-Ni	”
Catalysts – IMPRESS (FP6)	Al-Cr-Mo-Ni	”
Database development for titanium and nickel aluminides	Al-Nb-Ta-Ti-O	”
Management of database for elements on behalf of SGTE		”
Salts for novel lighting applications	Br-I-In-Na-Tl	”
Low temperature ionic liquids	C-Cl-H-N-O	”
GenIV Nuclear fuel	Na-O-Np-Pu-U	”
Salts for lighting applications	Dy-I-Na	”
Reprocessing of nuclear fuel	Cl-Pu-U	”

Interest	Material/system	Researcher(s)
Data for Mg alloys	Ce-Gd-Mg-Nd-Y-Zn-Zr	”
Salts for novel lighting applications	InX (X = Cl, Br, I) InX_3 (X = Cl. Br, I)	NPL (Alan Dinsdale & Hugh Davies) Ceravision (S.A.Mucklejohn)
Salts for phase change materials	H-K-Li-N-Na-O	NPL (Alan Dinsdale & Hugh Davies)
Comprehensive database development for oxide systems	Al-As-B-C-Ca-Cd-Co-Cr-Cu-F-Fe-H-K-Li-Mg-Mn-Na-Nb-Ni-P-Pb-S-Sb-Si-Sn-Te-Ti-V-Zn-Zr	NPL (John Gisby)
Development of database for inorganic industrial strength aqueous solutions up to 200°C	Br-Ca-Cl-Cu-Fe-H-K-O-N-Na-Ni-S-Zn-U	NPL (Hugh Davies)
Measurement of enthalpies of formation of chlorinated dioxins using a rotating bomb calorimeter	C-Cl-H-O	”
Study to facilitate development of new molten salt processes for metal extraction and carbon nanomaterial synthesis	LiCl-Li_2O	University of Cambridge (Carsten Schwandt, Derek Fray)
Development and maintenance of COST 531 lead-free solders database	Ag-Au-Bi-Cu-In-Ni-Pb-Pd-Sb-Sn-Zn	University of Leeds (Andy Watson)
Systems associated with high-temperature lead-free solders. HISOLD: COST MP0602	Bi-Cu-Sn Ag-Ga Ag-Ga-Sb	”
Contribution to MSI alloy programme	Al-Cr	University of Leeds (Andy Watson in association with Alexandra Khvan, University of Freiberg, Germany)
“	Ag-Sb-Sn	University of Leeds (Andy Watson in association with Gabriella Borzone, DCCI, U. di Genova, Italy)
“	Au-Cu-Ge-Ni	University of Leeds (Andy Watson & A.J. Scott, in association with Christian Leinenbach, EMPA, Switzerland and Gabriella Borzone, DCCI, U. di Genova, Italy)
	Co-Sm	University of Leeds (Andy Watson in association with Yuan Yuan, Central South University, Changsha, P.R. China & Gabriella Borzone, DCCI, U. di Genova, Italy)
Platinum group alloy systems	Al-Cr-Nb-Pt-Ru	University of Leeds (Andy Watson & Andy Scott)
	CaO-CuO/Cu2O-TiO2 Al_2O_3-CaO-CoO Pb-Pt-O TiO_2-Nb_2O_5/Cr_2O_3	University of Leeds (Girish Kale)
Sensors	$CaCu_3Ti_4O_{12}$	University of Leeds (Girish Kale & Andy Watson)
Atomic scale modelling of materials	$Dy_2Hf_2O_7$, $Ho_2Hf_2O_7$, $Er_2Hf_2O_7$	Imperial College, London (Robin Grimes)
High-temperature superconducting and multiferroic materials	Sr_2FeMoO_6, MgB_2, BiFeO3	University of Cambridge (Judith Driscoll)
	TiO_2-*M*	University of Bolton

Interest	Material/system	Researcher(s)
		(Guosheng Shao)
Non-stoichiometric phase, $Nd_2Ti_3O_{9-x}$	Nd_2O_3-TiO_2	University of Sheffield (Hajime Kinoshita)
M – transition metal, X – any other	Nb-Si-M-X	University of Sheffield (Claire Utton/Hajime Kinoshita/Panos Tsakiropoulos)
Electroceramic materials	$CaCu_3Ti_4O_{12}$, $Bi_{12}AO_{19.5}$ Sillenite-type phases related to γ-Bi_2O_3, $BaTiO_3$-based dielectrics, AO-La_2O_2-Nb_2O_5-TiO_2. Hexagonal Perovskites (microwave dielectrics). BaO-Bi_2O_3-Sb_2O_5-La_2O_3 (dielectrics), Bi_2O_3-WO_3 (Low temperature co-fired ceramics)	University of Sheffield (Derek Sinclair)
Stoichiometry of Pyrochlore Phases	Bi_2O_3-Sb_2O_5-ZnO, Bi_2O_3-Nb_2O_5-ZnO, Bi_2O_3-Ta_2O_5-ZnO	University of Sheffield (Tony West)
Doping $Zn_7Sb_2O_{12}$	ZnO-Sb_2O_5-MO:M=Ni,Mg,Cu, ZnO-Sb_2O_5-Cr_2O_3	,,
Ho & Nb-doped $BaTiO_3$ solid solutions and $BaTi_2O_5$	BaO-TiO_2-Ho_2O_3, Nb_2O_5	,,
Li-doped CoO and Co_3O_4		,,
Doped Li_2MnO_3 and related lithium battery cathode materials	Li_2O-CoO-MnO_2-NiO Li_2O-P_2O_5-Fe_2O_3	,,
Cu-Al-Ti nanostrcuture	Cu-Al-Ti	University of Sheffield (G. Moebus)
Irradiation induced phase separation in borosilicate glass		,,
Immobilisation of carbon-14 from reactor graphite waste by use of a self-sustaining reaction	C-Al-Ti-O	University of Sheffield (M. Ojovan)
Thermodynamic functions of zirconolite	Ca-O-Ti-Zr	University of Sheffield (M. Ojovan)
Alkali titanates	Ti-O-Na-K-Cl-F	UCL (Mark Tyrer)