

Materials Chemistry Committee Newsletter IOM3

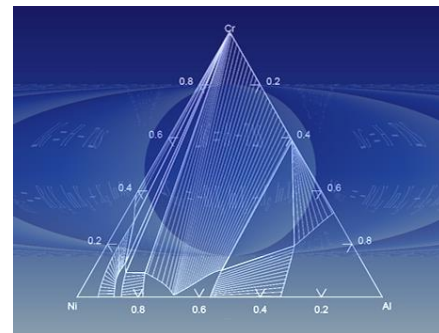
The Institute of Materials Minerals and Mining, 297 Euston Road,
London NW1 3AQ

www.iom3.org/materials-chemistry-committee

The Materials Chemistry Committee (MCC) is one of the 22 technical divisions and societies, groups and associations of Institute of Materials, Minerals and Mining (IOM3). Our aim is to provide UK industry and research organisations with consultancy and access to reliable up-to-date fundamental scientific information of phase equilibria and the thermodynamic properties of all classes of functional engineering materials, which plays a vital role in underpinning many spheres of materials science & technology.

Introduction

Welcome to the first edition of the Newsletter of the Materials Chemistry Committee (MCC) of the IOM3. The objective of this and future newsletters that will be published biannually is to keep those with keen interest in the Materials Chemistry up-to-date of the general activities and events of the MCC and about the new developments in the World of Materials Chemistry in particular. Features, links to interesting topical scientific and technical literature, key conference announcements and major developments in our field will all be included here, and together with the MCC Microsite delivered by IOM3, we will aim to offer a first point of contact for all the happening things in the world of



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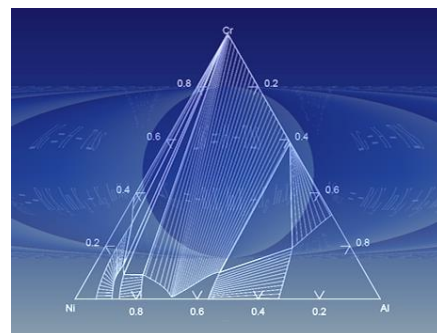
Dr. Mark Tyrer, Imperial
College London

Dr. Michael Rushton, Imperial
College London

“Materials Chemistry”. This will, of course, take time to achieve and I am sure that we will miss out inadvertently some things, so we would be grateful to learn of anything that you may think we should be covering by contacting directly the Editor-in-Chief of the newsletter. Our aim is to publish the MCC newsletters biannually. We hope that you will enjoy reading this first edition and find it useful. As always any comments, suggestions and contributions are always welcome.

Background

For those who do not know what the Materials Chemistry Committee (MCC) is, the MCC is one of the 7 technical committees that form the Materials Science and Technology Division of the IOM3. Formed in 1977 as “Phase Diagram Committee” of the then Institute of Metallurgists, its remit was to fulfil the UK's needs for phase diagram information. Membership comprised of the centres of academic excellence in Phase Diagram and thermodynamic investigations such as Universities of Birmingham, Cambridge, Leeds, Newcastle, Sheffield, and Imperial College together with industrial partners such as British Steel, GEC, Johnson Matthey, NPL and UKAE. The committee was also a founder member of Alloy Phase Diagram Commission (APDIC) involving 17 member organisations from around the globe. As the discipline evolved with time, the Institute of Metals became IOM3 and the Phase Diagram Committee was renamed as the MCC to serve wide range of interests in materials of different kind through experimental determination of phase diagrams and thermodynamic properties of phases to “Calphad” and *ab initio* modelling for serving materials processing and application needs of industries. The current constitution of the MCC still enjoys the membership of academia and industry while no longer focusing only on metals but on all types of inorganic materials. As a direct consequence of this the MCC is seen to be within the MSTD that strives to underpin the scientific and technological interests of several committees. The MCC is always open to welcome new members from academia and industry having wider scientific interests and expertise in order to successfully serve the UK's Materials community by providing support in every profession. Please visit <http://www.iom3.org/materials-chemistry-committee> for more information.



Dates for your diary

31st MSIT International Seminar on Heterogeneous Multicomponent Equilibria and 1st MSIT Winter School on Materials Chemistry
12 – 17 March, 2017
Kreuth, Germany

46th CALPHAD International Conference
11 – 16 June, 2017
Saint-Malo, France

231st ECS Meeting
May 28 – June 2, 2017
New Orleans, Louisiana, USA

37th Cement & Concrete Science Conference
11 – 12 September, 2017
UCL, London

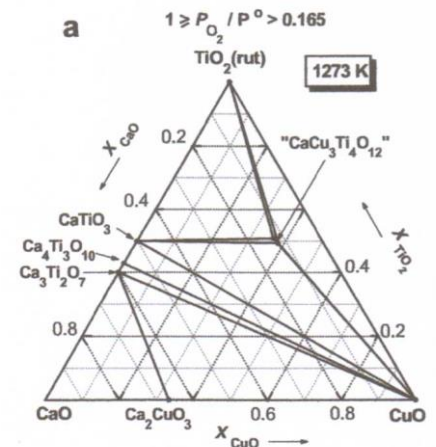
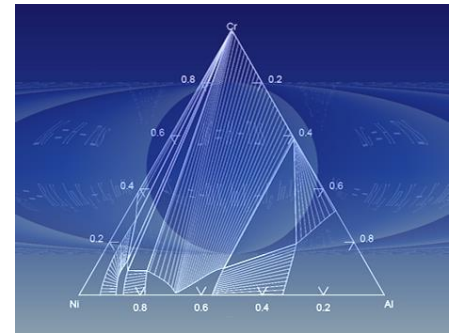
15th International Conference on Properties & Phase Equilibria for Product and Process Design,
12 – 16 May, 2019
Vancouver, Canada

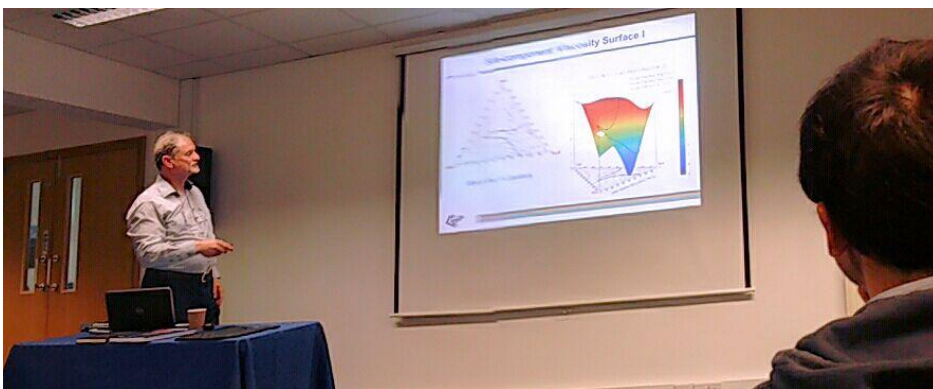
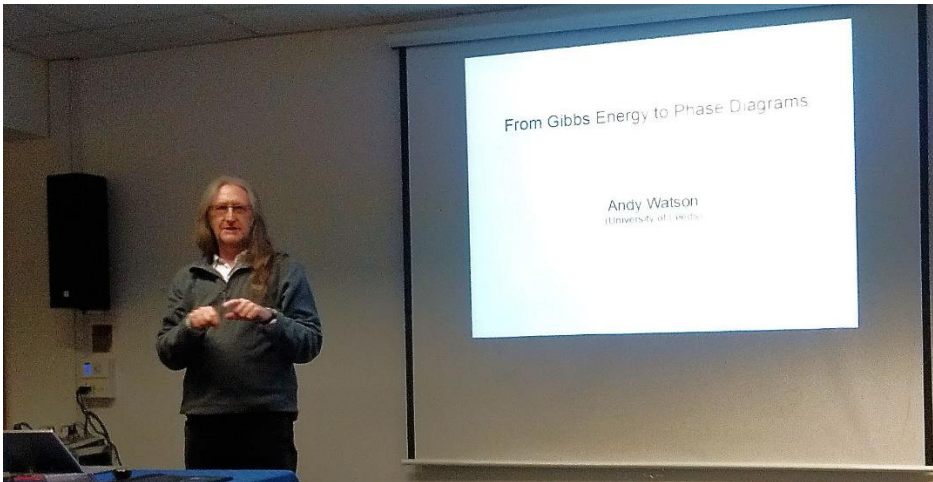
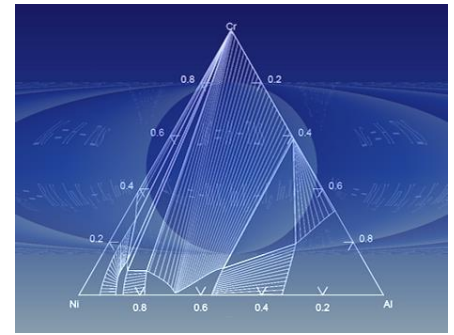
Mission

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. To this aim it provides a means by which critical assessment and experimental work carried out in various organisations in the UK can be discussed and undue overlap of experimental studies avoided. The committee will encourage international co-operation on phase diagram knowledge. It recognizes the vital role that reliable information on phase diagrams and the rates of approaches equilibrium plays in underpinning many spheres of materials science and technology. These include extraction, refining, processing and use of materials in traditional large scale industries as well as emerging applications and industries. Phase equilibrium and thermodynamics can also be used as a predictive tool to assist failure analysis and developing new sustainable materials for various technological applications[1].

News

The MCC recently organized highly successful 1st Hume – Rothery Seminar event sponsored by the Scientific Group Thermodata Europe (SGTE) from 16-18 January 2017 at the Riverside Conference Centre in the historic Roman town of Derby situated on the bank of river Derwent and most famously known as the home of Rolls-Royce aero-engines and Derby Litchurch Lane Works. The event was attended by more than 50 delegates both from industry and academia from UK, Germany and Sweden. The seminar proved to be thought provoking and an eye opener for some while scientifically stimulating for most. A total of 17 papers were presented of which 5 were on the application of phase equilibrium and thermodynamics for solving real world materials problems ranging from superalloys, slags and cements, discharge lamps and sensors for process monitoring and control. Selected photos from the event are displayed below.

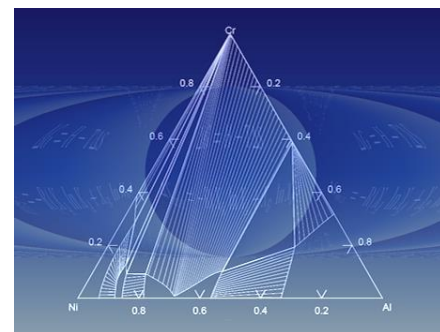




Items of interest and Dates for your diary

The 31st MSIT International Seminar on Heterogeneous Multicomponent Equilibria and 1st MSIT Winter School on Materials Chemistry will take place at Schloss Ringberg, Kreuth, Germany (<http://www.schloss-ringberg.de/home>) from Sunday the 12th to 17th of March 2017. As well as the usual workshops on the evaluation of binary and ternary alloy systems, a Winter School on Materials

Chemistry will run in parallel from the 12th to the 15th of March 2017. During this three day event, internationally renowned experts from the MSIT will be teaching subjects such as crystallography, computational thermodynamics and the principles of phase equilibria, and is aimed at those who may have only a bare knowledge of the subject area. It is anticipated that the winter school will become an annual event to run alongside the already successful MSIT seminars. For more information on the Winter School and MSIT seminar, visit <http://www.msiport.com/communities/msit/>



The 46th Calphad international conference will take place in St. Malo, France from 11th – 16th of June 2017. Topics for discussion will include all aspects of computational thermodynamics - modelling, assessment and applications. *Ab Initio* calculation is an increasingly popular subject area, and communications relating to experimental studies are also welcomed. Details can be found on the Calphad website www.calphad.org.

The Calphad conference will be immediately proceeded by the annual meeting of the members of APDIC (Alloy Phase Diagram International Commission), of which the IOM3 (represented by the MCC) is a founder member. APDIC was founded in 1986 with the aim of coordinating efforts in phase diagram research on a global scale, through the efforts of the research programmes of the individual members. A feature dedicated APDIC will appear in a future Newsletter. In the meantime, more information can be found at www.apdic.info.

Additional weblinks of interest

http://trc.nist.gov/metals_data/

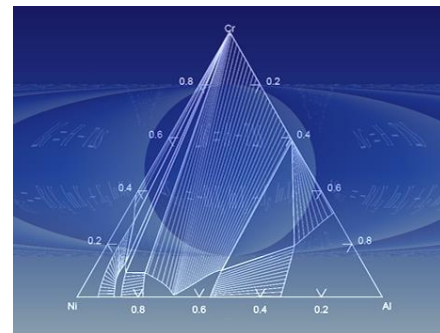
<http://sgte.net/en/>

<https://www.ucl.ac.uk/aim/conference-info/37ccs>

Bibliography

[1] K. Thomas Jacob, Chander Shekhar, Xiaogan Li, Girish M. Kale: Gibbs energy of formation of $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ and phase relations in the system $\text{CaO-CuO/Cu}_2\text{O-TiO}_2$, *Acta Materialia* 56 (2008)4798–4803.

[2] Seong-Pil Kang, Huen Lee: Recovery of CO_2 from Flue Gas Using Gas Hydrate: Thermodynamic Verification through Phase Equilibrium Measurements, *Environ. Sci. Technol.*, 2000, 34 (20), pp 4397–4400.



Advertisements



Post-Doctoral Positions

Properties of High Temperature Materials

Post-doctoral positions at the University of South Carolina are available to support a significant and growing effort on the development and assessment of novel high temperature materials including structural materials, nuclear fuels, and radioactive waste forms. Projects include understanding nano and framework materials for novel phases for waste wastes; developing thermochemical models for complex advanced fuels to allow assessment of behavior in service; and development representations of high temperature species transport in nuclear fuel materials. Specifically, there is a need for individuals to apply CALPHAD, and possibly first principles approaches to obtaining thermochemical properties and transport behavior in complex materials. In addition new approaches such topological and volumetric correlations are being applied, and the individual will have the opportunity to learn and apply these.

The positions require a PhD in chemistry, physics, materials science, or engineering, with experience in high temperature materials being helpful.

For further information, or to provide a CV for consideration, contact

Theodore M. Besmann, PhD
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MSIT Winter School on Materials Chemistry

12 -15 March 2017
Ringberg Castle
Kreuth
Germany

Organised by
MSI - Materials Science
International Services
GmbH.
Dr. Günter Effenberg
Dr. Andy Watson

In the frame of the
31st MSIT Annual
International Seminar
on Heterogeneous
Multicomponent Equilibria

Understanding Phase Equilibria is crucial to materials design, processing and is key to understanding behaviour. As a foundation of Materials Science its importance cannot be overstressed.

MSI and MSIT have organised this Winter School to inform and instruct on all things related to the study of phase equilibria, crystallography, thermodynamics (experimental and computational), corrosion, and magnetism.

Lectures at the Winter School are given by experts from MSIT who had years of experience, both in teaching and applying these methods.

Topics

- Phase Equilibria and Phase Diagrams
- Principles of Chemical Thermodynamics
- Crystallography
- Density Functional Theory
- Computational Thermodynamics

