

Materials Chemistry Committee Newsletter IOM3

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

www.iom3.org/materials-chemistry-committee

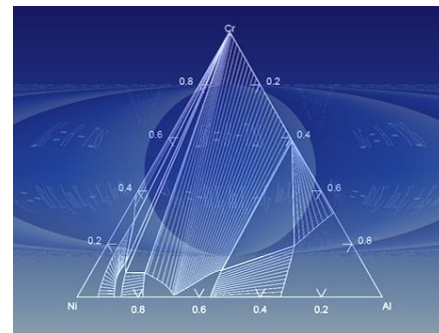
The Materials Chemistry Committee (MCC) is one of the 22 technical divisions and societies, groups and associations of Institute of Materials, Minerals and Mining (IOM3). Our aim is to provide UK industry and research organisations with consultancy and access to reliable up-to-date fundamental scientific 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.

Chairman's chat

Welcome to the second Newsletter of the Materials Chemistry Committee of the IOM3. I hope that you will find the contents of interest.

In issue 2, we start what we hope will become a regular feature on Committee Member profiles; so that you can see who we are and what our interests are. The first profile is that of our newest member, Prof. Shaowei Zhang who works in the Department of Engineering at the University of Exeter. We also offer congratulations to two of our members on taking new posts.

A regular feature of any Newsletter is a round-up of upcoming conferences and meetings, but we are including information of an



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University of Leeds

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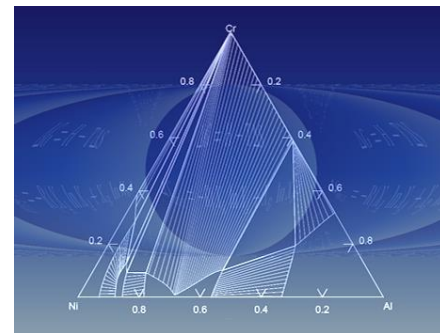
Professor Howard Stone,
University of Cambridge

Dr. Mark Tyrer, Imperial
College London

Dr. Michael Rushton, Imperial
College London

exciting new conference that the MCC is in the process of organizing - watch this space, and as always, keep your eyes on the MCC website.

We hope that with time, that through the Newsletter, along with the website and our LinkedIn group, the MCC will become your Information Point for all things related to Materials Chemistry, Phase Diagrams and Thermodynamic of Materials. We will introduce new features to future Newsletters, but if you have any suggestions or comments regarding Newsletter content, please let us know by emailing to matsiom3chem@gmail.com. We want you as the reader to feel that it is your Newsletter as well as ours and should be shaped to represent our interests.



Member profile

Prof. Shaowei Zhang has been a member of the committee since April 2017. Shaowei is currently a Professor and Royal Society Industry Fellow in the College of Engineering, Mathematics and Physical Sciences at the University of Exeter. Before moving to Exeter, he had worked for about 14 years in the Department of Materials Science and Engineering at the University of Sheffield as a postdoctoral research associate, an EPSRC advanced fellow and a Reader.



Shaowei has more than 25 years' of research and teaching experience. His main research interests are in the processing, microstructures and properties of a range of advanced materials, in particular, ceramics materials and composites. His current research topics include low temperature molten salt synthesis of nanomaterials, development of nanostructured low carbon composites for clean steel-making, novel synthesis of 2-D quantum dots for cancer diagnosis and treatment, exploration of 2-D nanocatalysts for hydrogen generation, and preparation of porous graphene for water-treatment. Other work includes preparation of oxide/carbide coatings and novel armour materials and development of ultrahigh-temperature ceramics.

In addition to research and teaching, Shaowei has acted as a consultant to more than 15 ceramics companies and their end-user companies.

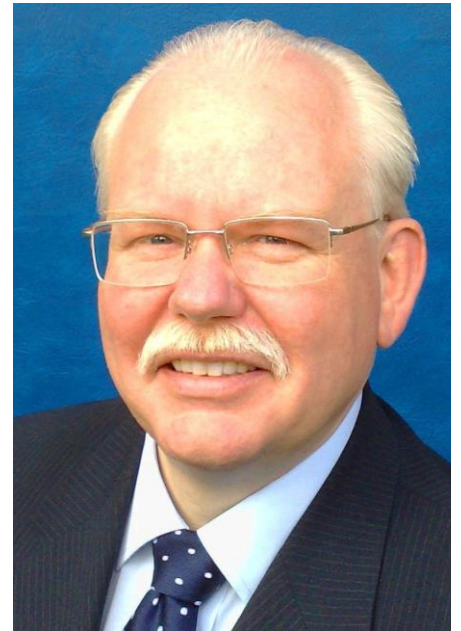
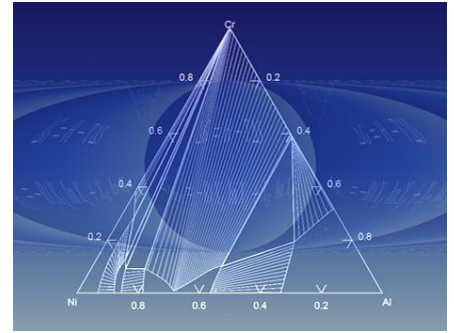
Appointments

Congratulations to Mark Tyrer, who joined Coventry University in December last year, where he has been appointed Executive Director of the Centre for Research in the Built and Natural Environment. Mark holds a personal chair in Geomaterials. His interests focus largely on cements, their use in environmental protection (particularly nuclear waste isolation) the resource-efficient use of materials in construction, the energetics and CO₂ footprint of cement production and the chemistry of blended cements. In addition, he works with stone and stone products, engineered and calcined clays and other minerals systems such as gypsum, titania and salts. Uniting much of this work, is his use of thermodynamic models to help better understand the mechanisms underlying material production, service life and durability.

He was appointed as a Director of the Association of Consulting Scientists in 2010. He currently serves on the British Standards committee B/516 (Cements), was appointed as a Director of the Association of Consulting Scientists in 2010 and recently served on the Concrete Society Expert Working Group on the Analysis of Hardened Concrete. In addition, he is a former chairman of the Construction Materials Group of the Society of Chemical Industry and current Chairman of the Cementitious Materials Group at the Institute of Materials, Minerals and Mining. Mark Tyrer was appointed as visiting Professor of Construction Materials at Coventry University in 2008 and received the IOM3 Pfeil award (2011) for work there on CO₂ reduction in the cement industry.

Coventry University will host the 38th Cement and Concrete Science meeting on the 10th and 11th September 2018 on behalf of IOM3, which will be Mark's final duty as group chairman, handing over the office to Professor Ian Richardson (U. Leeds) after serving the maximum six year term.

Alan Dinsdale has now joined BCAST, part of Brunel University London, as Professor of Materials Thermodynamics. His role within BCAST is mainly concerned with the development of critically assessed thermodynamic data for the Al-Fe-Mn-Si system with



particular emphasis on developing an understanding of the undercooling necessary to precipitate the ternary and quaternary intermetallic phases found during casting of commercial aluminium alloys. He has joined the theoretical modelling team which also has particular goals in the modelling of nucleation and interfacial properties.

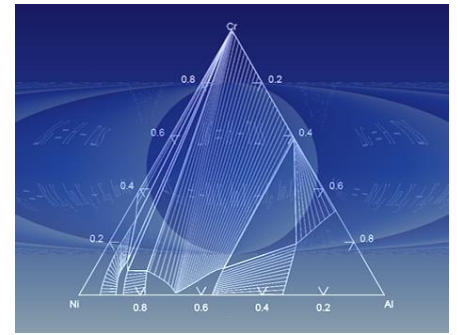
Alan also works part time for Hampton Thermodynamics, a private company formed with his old colleagues from the thermodynamic modelling group at NPL. His main interest there is the development of new thermodynamic datasets for the elements in conjunction with other members of SGTE, an area of work which is very close to his heart. After leaving NPL in 2014, Alan had worked for two years as part of a newly formed research group at the Moscow Institute for Steels and Alloys (MiSIS). This was a very rewarding experience for him and he maintains close working relationships with a number of friends and colleagues there.

Awards

The Materials Chemistry Committee is delighted that the IoM3 Hume Rothery prize for 2017 has been awarded to Prof Herbert Ipser.

Over a long career Herbert Ipser has established a huge international reputation in research into the thermodynamics and phase diagrams for metallic materials. His main research interests are thermochemistry and phase diagrams of metallic materials; thermodynamic, chemical and physical properties of intermetallics; ordering phenomena in liquids; and lead free solders. He has made major contributions in each of these fields.

Nearly all his work has been based at the University of Vienna where he studied for his PhD under the supervision of Prof. Kurt Komarek, although has also had significant experience working abroad and in particular during a two year spell between 1974 and 1976 at the University of Wisconsin with Prof. Austin Chang where he helped to compile a major review of phase diagram information for ternary copper-metal-sulphur systems. In Vienna he established a research group with unparalleled expertise in the measurement of thermodynamics properties such as the enthalpies of mixing or formation, vapour pressures and heat capacities, and studies of phase diagrams and the crystallographic properties of individual phases. This is reflected in



the long list of his publications and the outstanding quality of the output from his research group. The success of this group results partly from his ability to inspire his colleagues and his careful nurturing of students. He has always been much in demand as a lecturer at international conferences and symposia.

One of Herbert's great successes came in 2002 when he successfully initiated the European Project COST531 on lead free solder materials. This was later hailed as one of the most successful European projects ever bringing together research groups from 21 European countries in one collaborative venture. In a successor project MP0602 on high temperature lead free solders Herbert acted as the Austrian representative.

He has been in much demand in serving on various other committees during his career including those within the University of Vienna. In 2012 he became president of the Austrian Chemical Society. He has been heavily involved in the organisation of numerous conferences and symposia including "Thermodynamics of Alloys" in 1988 and 2004, High Temperature Materials Chemistry in 1994 and 2006 and the European Conference on Solid State Chemistry in 2015, all of which were held in Vienna.

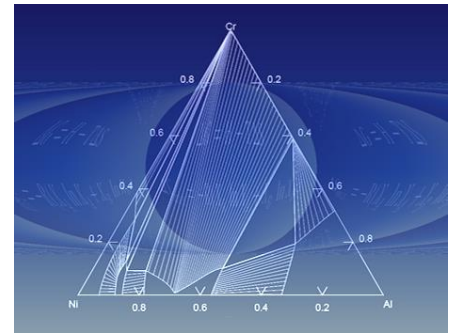
Note: The prize is awarded annually *in recognition of distinguished achievements concerned with phase relationships in metallic materials or non-metallic materials of metallurgical interest*. Both the nominee and the nominator may be members or non-members of the Institute and nationals of any country.

Conference Announcements

The 16th International Symposium on the Science & Technology of Lighting, LS16

This conference is organised by The Foundation for the Advancement of the Science & Technology of Light Sources (FAST-LS) in conjunction with the Centre for GaN Materials & Devices, University of Sheffield will be held in June 2018.

The LS Symposia have been held regularly since 1973 in venues in Europe, the USA and Asia. Their objective continues to be to provide an opportunity for the worldwide community of scientists and engineers engaged in both fundamental and applied aspects of lighting-related research and development to meet in an informal, non-commercial environment to gain a

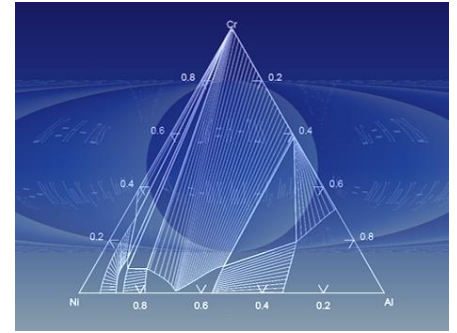


17 – 22 June 2018, Sheffield, UK



16th International Symposium on the Science and Technology of Lighting

comprehensive overview of current activity and issues in the field. There has always been a strong presence from the materials science community in these symposia as many of the constraints to light source efficiency are imposed by limitations of the properties of material, e.g. glasses, ceramics & metals. Recently the scope of the symposia have been extended to include environment aspects, human factors and non-visual effects of optical radiation. Session topics will include the following, but not limited to:



- Light Sources and Systems
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- Solid State Lighting systems (LED; OLED; Lasers)
- III-nitride semiconductors for visible lighting
- Novel & legacy light sources
- Light source materials
- Lighting controls and electronic control gear
- Smart lighting systems
- Human-factors in Lighting
- Physical & psychological effects of light
- Lighting & the visual environment
- Lighting design
- Applications and Technologies
- Biological effects of optical radiation
- Lighting for transport
- Lighting for Smart Cities
- Lighting for horticulture & animal husbandry
- Lighting metrics & metrology
- Environmental impacts
- Light pollution
- Impacts on eco-systems
- Lifecycle Assessment & Lifecycle Costs
- Regulations, guidelines & public policies

The papers published in the proceedings of the symposium will be referenced by internationally recognised databases of peer-reviewed literature such as IEEE Xplore, Scopus and Web of Science.

The first LS16 announcement was published in June. The second announcement giving details of the symposium website, registration, fees and submission of papers will be distributed in November.

1 – 5 October, 2018, Seoul,
South Korea

TOFA 2018

Thermodynamics of Alloys Conference (TOFA 2018)

The biennial TOFA conference will take place at Korea University, Seoul, South Korea, from October 1st to the 5th, 2018. The first 'Discussion Meeting on the Thermodynamics of Alloys' took place in Austria in 1988, and has been held every two years since then at venues in many parts of the world. Although originally concerned with thermodynamics, phase equilibria has always been an important topic. Originally, discussions were focussed mainly on experimental developments but more recently, Calphad modelling has played a prominent role in discussions. A brief history of the meeting can be found here:

<https://link.springer.com/article/10.1007/s11669-015-0362-x>

No details of the next meeting are available at present but a dedicated webpage will be available in due course.

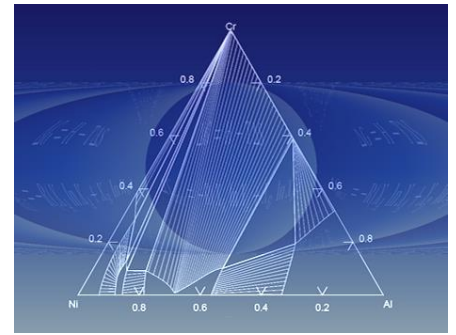
Phase Equilibria and Thermodynamics for the UK - AToMS2018

Following on from the success of the 1st Hume-Rothery seminar, which was held in January 2017, the MCC has decided to augment this biennial event with an annual conference on the Phase Equilibria and Thermodynamics of Materials. Feedback from the Hume-Rothery seminar was very good, and it highlighted an interest in the UK Phase Diagram and Thermodynamics community for a meeting to discuss current research in addition to the teaching/demonstration style of the Hume-Rothery seminar.

The **1st Annual Thermodynamics of Materials Symposium (AToMS2018)** will take place on the **26th June 2018** hosted at the **University of Sheffield**. This one day meeting will bring together people working in the areas of phase equilibria and thermodynamics and associated fields. The aims of the meeting are to discuss current research (both experimental and computational) and to develop a UK network of scholars and practitioners with an interest in phase equilibria and thermodynamics.

Oral and poster contributions from participants are invited. Topics include, but are not limited to:

Experimental phase equilibria, thermodynamics and kinetics
Thermodynamic and diffusion modelling
Ab-initio (first-principles) calculations
CALPHAD assessments and database development



26 June, 2018, Sheffield, UK

AToMS2018

Applications of phase equilibria and thermodynamics in materials science, chemistry and geology

A formal call for papers will be issued at the end of 2017.

This conference is jointly organised by the IOM3 Materials Chemistry Committee and the University of Sheffield and sponsored by CALPHAD Inc.

For further information please contact Dr Claire Utton c.utton@sheffield.ac.uk or Dr Andrew Watson

6th APDIC World Round-Robin Seminar

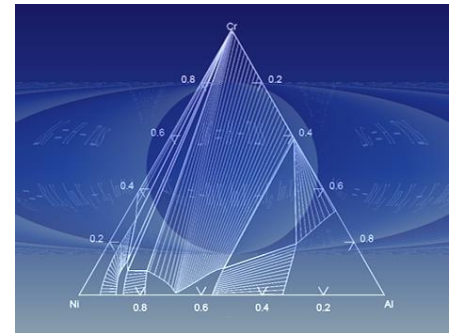
The 6th APDIC World Round-Robin Seminar (WRRS) on Phase Diagrams and Thermodynamics will be hosted by MSI GmbH and will take place at Schloss Ringberg in the beautiful Bavarian Alps near Tegernsee in Germany from 11th to the 14th of February, 2018, running in parallel to the annual MSIT meeting on Heterogeneous Equilibria. Previous seminars have been held in Moscow, Rio de Janeiro, Montpellier, and in 2012 the meeting was held in London, hosted by the MCC at 1 Carlton House Terrace.

The APDIC World Round Robin Seminar is organized by APDIC (Alloy Phase Diagram International Commission), of which the IOM3 is a founding member. As part of its remit to promote both quality standards for phase diagram evaluations and the application of phase diagrams in industry and academia, APDIC organises educational seminars on phase diagrams aimed at beginners and experts alike. The lecturers are selected from the APDIC membership or chosen by APDIC as well-known experts in their respective fields, and they provide a systematic knowledge of phase diagrams starting from the fundamentals of how to read a phase diagram to up-to-date application in designing new materials such as for functional and electronic devices. The seminar content will also include a 'Hands-on' element. More information is available from <http://www.msiport.com/msit-school/next-msit-school-wrrs/>

News

Metallurgical and Materials Transactions E to Merge Content

Content previously published in Metallurgical and Materials Transactions E: Materials for Energy Systems (MMTE) will merge into



11 – 14 February, 2018,
Schloss Ringberg, Germany

6th APDIC WRRS



Metallurgical and Materials Transactions A (MMA). Principal Editor Tresa Pollock discusses the changes to these publications.

Read more at http://www.tms.org/portal/ABOUT/News_Media/TMS_News/Current_TMS_News/portal/About/News_Media/TMS_News_Current.aspx?hkey=2832c964-7404-4547-bf58-40b3e69c2f3e&_z=tdshN81&_z=0d14#story1

Abstract Deadline Extended for TMS-FEMS Symposia

TMS and the Federation of European Materials Societies (FEMS) have extended the abstract submission deadline for the two special symposia the societies are jointly planning for the TMS 2018 Annual Meeting & Exhibition. Abstracts are due September 30.

Read more at http://www.tms.org/portal/ABOUT/News_Media/TMS_News/Current_TMS_News/portal/About/News_Media/TMS_News_Current.aspx?hkey=2832c964-7404-4547-bf58-40b3e69c2f3e&_z=tdshN81&_z=0d14#story2

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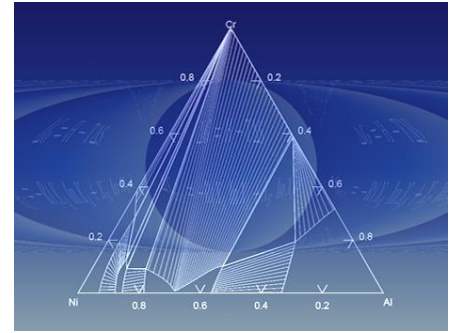
SGTE bibliographic database

ThermDoc – a compilation of references on phase diagrams and thermodynamic properties

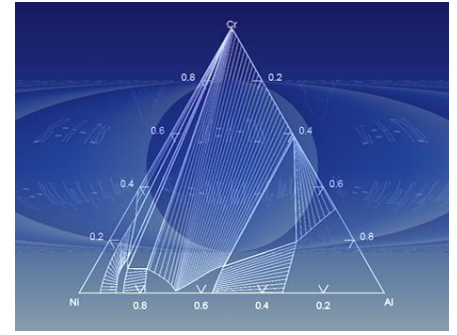
ThermDoc is a bibliographic database of articles published in the scientific literature covering thermodynamic data and phase equilibria of inorganic and metallurgical systems. It is developed and maintained by members of SGTE and is updated twice a year. Coverage of the references for a particular system is good for articles published since about 1970. The current **ThermDoc** database has more than 90000 references. About 1000 new references are added each year.

There are two software packages available which support ThermDoc and provide means of retrieving references for selected systems. **Papyrus** is the older software package and, while it is no longer under development, it offers a degree of flexibility in searching for references and provides a facility for a user to create and manage his own bibliographic database.

The more recent software package, **Biblio**, is under continuous development. Although, at the moment, it has more limited functionality, it does have the advantage that it is more portable and easier to implement.



Both software package, **Papyrus** and **Biblio**, and the ThermDoc database are available for Windows at no cost. Each record in the database consists of: Title, Author's names, complete bibliographic references and the systems covered.



Search Results

Current Database: D:\work\papyrus\2010\ThermDoc\Tb.dat

Number of references for Cu₂Zn = 33

File: Landa-Someren et al 1993, Thermodynamic Properties Of Inorganic Materials, P 76-80, Springer-Verlag 2005
Cu₂Zn

Y.C. Liu, J.B. Wan, Z.M. Guo, J. Alloy Compounds, Volume 465, Issues 1-2, Pages 296-298 (5 October 2008)
"Intermediate Decomposition Of Metastable Cu₂Zn Phase In The Solided Sn-Ag-Zn-Cu Interface"

T. Hergert, S. Heikamp, F. Dinkel, M. Kneip, G. Wenzel, Z. Cizilek, M. Kopy, J. Alloy Compounds, Volume 487, Issues 1-2, Pages 103-102 (13 November 2009)
"Experimental Determination Of Solid-Solid And Solid-Liquid Interfacial Energies Of Solid (Cu₂Zn) In The Zn-Cu Alloy"

Zhou, W., Liu, W., P. Heilmann, 13 (5), 922-928 (2010)
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U. Sprock, M. Kays, E. Cadel, N. Matalid, A. Unger, J. Alloy Compounds, Volume 491, Issues 1-2, Pages 142-148 (18 February 2010)
"Investigation Of The Effect Of Solidification Processing Parameters On Microstructure And Determination Of Thermo-Physical Properties In The Zn-Cu-Pb-Ti System"

Jiang Wang, Hongshu Xu, Shunfeng Zhang, Lian Zhang, Yong Du, Wenzong Zhang, Shuhong Liu, Feihong Wang, Zhi-Hai Liu, CALPHAD, Volume 35, Issue 2, Pages 181-193 (June 2011)
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Atsu Berrak, Edgar Dachs, Martin Schuster, Aleksandar Paunovic, Marko E. Miler, J. Chem. Thermodyn., 2014, 71, 150-162
"The vibrational and configurational entropy of gamma brass"

Song-Min Yung, Hyeon-Ming Yoo, Rainer Schmid-Fetzer, CALPHAD, 2015, 51, 226-232
"Thermodynamic assessment of the Ni-Cu-Zn system, part I: Cu-Zn binary system"

A. Kinsinger, H. Inayat, R. Schmid-Fetzer, A. Grosse, R. Waser, M. D. Hoesel, CALPHAD, 2015, 51, 369
"The assessment of the Ni-Cu and Cu-Zn systems with respect to the gamma brass phase"

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