

Case Statement:

RDA Working Group International Materials Resource Registries  
(WG IMRR)

## **1. WG Charter:**

### 1.1 Mission

As a domain, Materials Science and Engineering (MSE) is exceptionally broad and interdisciplinary with its origins most directly from metallurgy, ceramics and polymer science, but also with important ties to other disciplines such as physics, chemistry, chemical engineering, geology, electronics, optics, and biology. As a global community, MSE is expanding rapidly worldwide through the establishment of large, multi-institutional academic research centers, government labs, industrial consortia, and computing facilities. MSE researchers often need to answer complex questions such as “What structural properties and processing methods are required to develop new lightweight materials that significantly improve fuel efficiency yet meet safety standards satisfied by traditional materials in use today?” To this end we have seen the creation of programs such as the Materials Genome Initiative (MGI) in the US that aim to decrease the cost and time to develop new materials by a factor of two through more effective discovery, access, and interoperability of experimental and simulation data. However, finding the latest materials data and resources to answer such questions amidst this rich diversity and accelerated growth is an increasingly difficult and time-consuming endeavor.

In response, the RDA/CODATA Materials Data, Infrastructure, and Interoperability Interest Group (MDII IG; co-chairs James Warren, NIST, and Laura Bartolo, Northwestern University) in collaboration with materials science professional societies, proposes to create its first Working Group focused on developing the metadata standards required to establish a network of International Materials Resource Registries (IMRR) in key sub-domains and regions.

Developing a successful international materials science resource registry requires a combination of technical and political process. As an outgrowth to discussions held in MDII IG working sessions and based on knowledge of the materials community, MDII IG proposes core members for its Working Group. The core members would be comprised of “doers” in the materials and cognate communities to identify those in their organizations who need to be involved. CVs have been collected and are included in this proposal to demonstrate MDII IG’s beliefs that leadership is required from a diverse set of organizations and that these people hold positions to ensure action will follow.

As an Interest Group, MDII brings forward its Working Group proposal to TAB because RDA, by its nature, provides a platform for building international consensus. MDII IG believes that RDA offers the leverage and vehicle needed to

embrace communities who want to build data discovery, access, and interoperability capabilities under its aegis.

A resource registry is a system that harvests and makes searchable high-level metadata descriptions of resources held by data repositories, archives, organizations, websites, and services to aid scientists in industry, universities, and government labs in the discovery of data relevant to their research and work interests. The IMRR WG will be comprised of an international committee representing different regions and sectors, including Asia, Europe, and North America with MDII IG Co-Chairs as ex-officio members. A Convener will be responsible for coordinating the activities of the Working Group and will facilitate interactions with other closely-related Interest and Working groups.

Invited core members include:

Convener:	Chandler Becker	ODI, MML, NIST	US
Core Members:	Scott Henry	ASM Int'l *	US
	Brian Matthews	STFC	UK
	Debbie Mies	Granta *	UK
	Raphael Ritz	EUDAT/NOMAD	EU
	Yibin Xu	NIMS	JP
	Haiqing Yin	Univ Sci & Tech	CN
Ex-Officio	Laura Bartolo, Co Chair, MDII IG		
	James Warren, Co Chair, MDII IG		

The proposed materials resource registry would develop a common framework for high level description of materials resources, including data, simulations, software, and instrumentation with respect to open standards to support materials data sharing as well as collaborative efforts. The materials resource registry work would determine minimal metadata for materials resources listed in the registries such as data collections, services, and tools. The registry work would facilitate access, discovery, use, and re-use through technical and social infrastructure development with the community: metadata, vocabularies, formats, and best practices. Working in close collaboration with complementary RDA Working Groups and Interest Groups (e.g., Domain Repositories IG, Metadata IG and WG, Photon Neutron Science IG, and Metadata Standards Catalog WG), the IMRR would serve as a potential test bed for integration of emerging RDA products that meet the needs and interests of the materials science community.

Given the broad reach, the multiple sub-domains and international efforts of MSE, and the substantial global materials data initiatives, the timing is

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\* Granta is a private, independent company partially owned by ASM International.

opportune for the materials science professional societies to collaborate with the RDA on an international materials resource registry project. The US National Institute of Standards and Technology (NIST) has a leadership role in MGI and the international MSE community and is willing to provide technical support for this initiative with RDA, international materials research organizations, and professional societies.

## 1.2 Stakeholders

The proposed establishment of a network of materials resource registries would connect with key stakeholders across the international materials communities:

- Individual Level: scientists in industry, universities, and government labs
- National Level: centers and consortia in industry and universities, professional societies in materials science and engineering
- International Level: CODATA, other joint international initiatives
- Cognate Areas: Interdisciplinary ties across STEM, such as with the Photon/Neutron IG

## 1.3 Goals (See section 4, Work Plan and Operation for more detail)

### 1.3.1 Short term (12 to 18 Months)

- Define and build consensus around minimum required metadata for materials science data discovery
- Deploy metadata schema using pilot registry infrastructure developed by NIST
- Validate with materials science data collections at organizations participating in the Working Group

### 1.3.2 Long term (Post 18 Months)

- Build, Grow, and Maintain a Social/Technical Global Network of IMRRs

## 2. Value Proposition, Beneficiaries, and Key Impacts:

### 2.1 Value Proposition

The IMRR would consist of high-level resource descriptions that would be harvested into a federated registry using the Open Archives Initiative Protocol for Metadata Harvesting (OAI-PMH). Its establishment would promote:

- Discovery and sharing of materials resources
  - Organizations (University, Research Group, Government)
  - Data Collections (Repository, Project Archive, Database)
  - Datasets
  - Services
  - Informational Sites
  - Software
- Bridging the gap between distributed resources and users
- Support for collaboration and reuse of data and resources

- Access to complex, heterogeneous, distributed data for many users

## 2.2 Beneficiaries

The IMRR would benefit its stakeholders (1.2) as well as the international STEM communities. The process for building out sufficient, but not excessive, metadata to serve data discovery needs in materials science will be documented and can serve as both a social and technical model for initiatives in other disciplines.

## 2.3 Key Impacts

- Establish a common, framework for high level description of materials resources.
- Facilitate access, discovery, use, and re-use of a wide range of distributed materials resources.
- Encourage materials data sharing as well as support collaborative efforts.
- Improve the return on investment in materials science data.

## 3. Engagement with existing work in the area:

The IMRR would build upon and continue engagement with:

Research Data Alliance (RDA)

- Its social and technical bridges to enable open sharing of data.
- Its vision of researchers and innovators openly sharing data across technologies, disciplines, and countries to address the grand challenges of society.

OpenAIRE (Europe)

- Discovery of publications, projects, data, people, organizations, and data sources.
- Open access to publications and datasets

Virtual Observatory (VO)

- Discovery of datasets from thousands of astronomical collections known to the VO over wide areas of the sky.

The VO and its governing body, the International Virtual Observatory Alliance, would serve as an important model of a federated data environment for conducting research on the network:

- Federates thousands of archives, databases, and services around the world
- Open interoperability standards integrate community web tools, web services, desktop apps, and software libraries
- Discovery Framework (part of VO – set of standards)
  - General data model and standards that supports discovery of a broad variety of resources
  - Datasets, records in databases, services, useful websites
  - Extensible metadata model that can be customized for different types of resources
  - Allows data providers to expose collection-specific (non-standard)

- metadata into discovery process
- Allows data providers to support standards incrementally
- Simple registration to inform world that the website exists
- Can add further support for standards as able to increase visibility within federation

#### **4. Work Plan and Operation**

The scope of this activity would fit well into an 18-month timeline. Schedule milestones are as follows:

##### **4.1 Recruit Domain Experts, Survey Landscape and Begin Discussions (M 1-3)**

Month 1 (Jan'16): recruit domain specialists to participate in the WG

Month 2 (late Feb/early Mar'16): initiate discussions about conducting a survey of existing materials science data providers in order to build on existing experience and expertise; develop 20 typical data discovery queries to inform metadata discussions

Month 3 (March – April '16): hold meeting to draft first version of metadata extensions to Dublin Core

##### **4.2 Disseminate Preliminary Findings, Solicit Feedback and Convene 2<sup>nd</sup> Meeting (M 4-8)**

Months 4-8 (Apr – Aug '16): disseminate draft to the materials science community, both within and external to RDA, and solicit feedback

Month 8 (Aug'16): hold second two-day meeting to refine metadata extensions and establish implementation pilot program (e.g., NIST Materials Repository, NDS Materials Data Facility, and others to be determined within the WG)

##### **4.3 Implement and Test Pilot MSE RR, Prepare initial Documentation and Revise (M 8-16)**

Months 9-12 (Sept – Dec '16): implement pilot federated registry and recruit testers/evaluators; evaluate granularity issues (at what level does one aggregate service descriptions?) and write best-practices guideline document

Months 13-15 (Jan – Mar 17): fine tune metadata definitions and document metadata development process: what worked well, what did not; expand the content of the pilot registry

##### **4. 4 Prepare Final Report (M 16-18)**

Months 16-18 (Apr -- Jun'17): prepare final document for delivery to RDA at P10

#### **5) Adoption Plan:**

The deliverable for this Working Group would be a document defining a minimum level of metadata needed to facilitate discovery in the materials sciences. At the core of the metadata definition would be the Dublin Core metadata, long established as useful for key provenance information. But similar to the Virtual Observatory Resource Metadata (<http://www.ivoa.net/documents/latest/RM.html>), the IMRR metadata would include domain-specific extensions to help identify key types of materials data (polymers, ceramics, semi-conductors, nanomaterials, etc.). These metadata extensions would be developed through the coordinated work of domain experts spanning the primary materials science sub-disciplines working together with metadata design experts. The IMRR would also be foundational work for the eventual deployment of more detailed data discovery and utilization services, e.g., using RDF and Linked Data. NIST, for example, through the Materials Genome Initiative and the Office of Data and Informatics, Material Measurement Laboratory, would be interested in supporting such a pilot.

## 6) Initial Membership

### 6.1 Leadership

- International representation of key regions
- Leadership ties with regional/national materials communities
- Close ties with IG MDII
- brief CVs in Appendix

### 6.2 Participation/Interested Members

The WG would request international assistance and participation from major materials science and engineering data centers with pilot implementations to help validate the choices of metadata elements.

- identify and establish international hubs for regional/national resources

## 7. References

Hanisch, RJ et al. "The Virtual Astronomical Observatory: Re-engineering Access to Astronomical Data" *Astronomy and Computing*, June 2015, 11, Part B: 190–209

Youssef, S et al. "Materials Data Curation System" DOD AFRL Materials Research Collaborative Environment Workshop, July 2015, Dayton, OH.

## 8. Appendix

CVs of individuals who have agreed to be on the WG

Chandler Becker	ODI, MML, NIST	US
Scott Henry	ASM Int'l *	US
Brian Matthews	STFC	UK
Debbie Mies	Granta *	UK
Yibin Xu	NIMS	JP
Haiqing Yin	Univ Sci & Tech	CN

## Curriculum Vitae

### Dr. Chandler A. Becker

**Affiliation** National Institute of Standards and Technology  
Office of Data and Informatics, Material Measurement Laboratory  
100 Bureau Dr.  
Gaithersburg, Maryland, USA

**Phone / Fax** 301-975-5344 / 301-975-4553

**e-mail** [chandler.becker@nist.gov](mailto:chandler.becker@nist.gov)

### Education and Professional Experience

#### Education:

1999: Bachelors of Science with Departmental Honors, The College of William and Mary, Williamsburg, Virginia, USA

2006: Doctor of Philosophy, Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois, USA

#### Positions:

1999-2001 Analyst, High Performance Technologies, Inc., Reston, Virginia, USA

Since 2006 Materials Research Engineer, National Institute of Standards and Technology, Gaithersburg, Maryland, USA

### Honors and Awards, Professional Activities:

2015 NIST Sigma Xi Katharine B. Gebbie Young Scientist Award

2011 Bronze Medal for Superior Federal Service, NIST / Department of Commerce.  
For development of the NIST Interatomic Potentials Repository

2008 Best Paper Award (one of three), World Materials Research Institutes Forum  
Workshop for Young Scientists, Tsukuba, Japan.

2006-2008 National Research Council NIST Postdoctoral Research Associateship

2005 Best Student Poster Award, Frontiers in Solidification Symposium,  
TMS Annual Meeting

2001-2002 Walter P. Murphy Fellowship, McCormick School of Engineering,  
Northwestern University

2015 Review panel member, US Department of Energy INCITE program

2015 Programming committee, Foundations of Molecular Modeling and Simulation  
(FOMMS) conference

2014 Co-organizer, Computational Modeling and Simulation of Advanced Materials  
for Energy Applications Symposium, TMS 2014 Annual Meeting

2008 – 2014 Organizer or co-organizer of the annual NIST Workshops on  
"Atomistic Simulations for Industrial Needs."

Since 2011 Member, TMS committee on Integrated Computational Materials Engineering (ICME)

Since 2011 Advisory Board Member, Knowledgebase of Interatomic Models (KIM) project

Journal Reviewer, including Physical Review Letters, Physical Review B, Physical Review E, CALPHAD, Modelling and Simulation in Materials Science and Engineering, and conference proceedings.

#### **Selected Publications – Chandler A. Becker**

- S. R. Kalidindi, J. Gomberg, Z. T. Trautt, and C. A. Becker, Application of data science tools to quantify and distinguish between structures and models in molecular dynamics datasets, *Nanotechnology*, 26, 344006 (2015).
- Z. T. Trautt, F. Tavazza and C. A. Becker, Facilitating the selection and creation of accurate interatomic potentials (force fields) with robust tools and characterization, *Modelling Simul. Mater. Sci. Eng.*, 23, 074009 (2015).
- C. A. Becker, J. Ågren, M. Baricco, Q. Chen, S. A. Decterov, U. R. Kattner, J. H. Perepezko, G. R. Pottlacher, and M. Selleby, Thermodynamic modelling of liquids: CALPHAD approaches and contributions from statistical physics, *Phys. Status Solidi B*, 251, 33–52 (2014).
- C. A. Becker, F. Tavazza, Z. T. Trautt, and R. A. Buarque de Macedo, Considerations for choosing and using force fields and interatomic potentials in materials science and engineering, *Curr. Opin. Sol. State Mat. Sci.*, 17, 277–283 (2013).
- C. A. Becker, F. Tavazza, and L. E. Levine, Implications of the choice of interatomic potential on planar faults and surface properties in nickel, *Phil. Mag.*, 91, 3578–3597 (2011).
- E. B. Tadmor, R. S. Elliott, J. P. Sethna, R. E. Miller, and C. A. Becker, The potential of atomistic simulations and the knowledgebase of interatomic models (KIM), *JOM*, 63, 17 (2011).
- C. A. Becker and M. J. Kramer, Atomistic comparison of volume-dependent melt properties from four models of aluminum, *Modelling Simul. Mater. Sci. Eng.*, 18, 074001 (2010).
- M. I. Mendeleev, M. J. Kramer, C. A. Becker, and M. Asta, Analysis of semi-empirical interatomic potentials appropriate for simulation of crystalline and liquid Al and Cu. *Phil. Mag.*, 88, 1723–1750 (2008).
- C. A. Becker, J. J. Hoyt, D. Buta, and M. Asta, Crystal-melt interface stresses: atomistic simulation calculations for a Lennard-Jones binary alloy, Stillinger-Weber Si and Embedded Atom Method Ni, *Phys. Rev. E*, 75, 061610 (2007).
- C. A. Becker, D. Olmsted, M. Asta, J. J. Hoyt, and S. M. Foiles, Atomistic underpinnings for orientation selection in alloy dendritic growth, *Phys. Rev. Lett.*, 98, 125701 (2007).



# Scott D. Henry

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## Experience

**ASM International**, Materials Park, Ohio ([www.asminternational.org](http://www.asminternational.org))

**2014-present**      **Director, Content and Knowledge Based Solutions**

*Role and responsibilities*

- Direct strategic planning, content development, and business management for reference and scholarly publications and professional education programs
- Direct the strategic development of materials data programs, including the Computational Materials Data Network ([cmdnetwork.org](http://cmdnetwork.org))
- Principal investigator: Structural Materials Data Demonstration Project (National Institute of Standards and Technology cooperative research project), 2013-2015
- Principal investigator: NIST Center for Hierarchical Materials Design (ASM subcontract to Northwestern University), 2014-present

**2007-2014**    **Senior Manager, Content Development and Publishing**

**2005-2006**    **Senior Product Manager**

**2004-2005**    **Senior Manager, Product Development, Publications**

**1997-2004**    **Assistant Director, Reference Publications**

**1989-1997**    **Various editorial content development and production roles**

## Education

**M.A.**, University of Illinois, Champaign-Urbana, IL, 1989

**B.A.**, Ohio State University, Columbus, OH, 1987

## Publications (selected)

- S.D. Henry, L.A. Berardinis, Computational materials data: an update. *Metallography, Microstructure, and Analysis*, Vol 4, Issue 6 (December 2015), pp 455–458, doi:10.1007/s13632-015-0248-7.
- S.D. Henry, L.A. Berardinis, A review of materials data infrastructure projects, in *Proceedings of the 3rd World Congress on Integrated Computational Materials Engineering* (TMS, 2015), pp 277–284
- S.D. Henry et al, Structural materials data demonstration project—resource for thermal process modeling, in *Proceedings from the 5th International Conference on Thermal Process Modeling and Computer Simulation* (ASM International, 2014, p 96
- S.D. Henry, Materials data for modeling. *Metallography, Microstructure, and Analysis*, Vol 1, Issue 2 (2012), pp 77–78. doi:10.1007/s13632-012-0020-1.

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# CURRICULUM VITAE

**Dr. Brian Matthews, FBCS**

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## Education:

1990 - 1993	Dept. of Computing Science, University of Glasgow.	Ph.D, Computing Science (awarded 1997) <i>Topic: Order-Sorted Term Rewriting Systems</i>
1986 - 1988	Dept. of Computing, Imperial College, University of London.	M.Sc. Foundations of Advanced Information Technology (Part-time).
1983 - 1986	Dept. of Mathematics, University of Bristol.	B.Sc. Mathematics (2-i )

## Employment

2014 -	Programme Manager, Scientific Computing Department, STFC	Leads the programme of work for SCD with partners in STFC and external facilities.
2003 - 2014	Group Leader, Scientific Computing Department, STFC	Leader of a research and development group within SCD, e-Science and Information Technology departments in STFC
2002-2015	Lecturer (part time), Oxford Brookes University	Lecturing on MSc on Web Technologies, Dept of Computing and Mathematical Science.
1986-2003	Researcher, CCLRC	R&D in computer science and information technology

Brian is **the Programmer Manager for the SCD Facilities Programme**, a £2M programme of work with some 30 staff across the department. He is responsible for the strategic development of the programme, providing both technical foresight and direction, and its planning resourcing and delivery. He sits on the senior management committee of the Scientific Computing Department.

Brian led the **Research Data Group** at the Scientific Computing Department of the Science and Technology Facilities Council <http://www.scd.stfc.ac.uk/>, a group of up to 30 software engineers and information specialists. The group undertakes research and development into areas including information management (including data management, library systems, semantic web, and data curation), and scientific visualisation and analysis tools in support of the scientific facilities of the STFC and its user communities. It is supported by internal STFC funds, and a variety of UK funding bodies (including JISC and research councils), and European Commission funded projects. The group works closely with UK academic sector, both in computing science research and in the wider science application community.

Brian has also held a part-time lectureship at Oxford Brookes University since 2002, teaching XML and Semantic Web on MSc on Web technologies, and supervising PhD students within computer science.

## Selected Projects:

Brian Matthews has extensive experience on a wide range of projects within STFC e-Science and its predecessor organisations. A selection of relevant recent projects include:

- **NFFA-Europe (2015-2018): EC-Infrastructures project on data sharing infrastructure within Nano-technology.**
- **PanData-Open Data Infrastructure (2011-14): EC Infrastructures project on developing a common data management infrastructure across European Neutron and Synchrotron Facilities**
- **SCIDIP-ES (2011-14): EC Infrastructures project developing preservation infrastructure in earth science projects**
- **SCAPE (2011-14): EC ICT project developing scalable digital preservation systems across European memory institutions.**
- **ENGAGE (2011-14): developing an information portal for open public data within the EC.**
- **APARSEN (2011-15): an EC funded network of excellence in digital preservation.**
- **CONTRAIL (2010-13): EC ICT project developing a elastic federated cloud systems**
- **XTREEMOS (2006-10) EC ICT project developing a grid-based operating system,**
- **Data Portal and ICAT (ongoing ):** STFC's system for cataloguing, browsing and distributing scientific data produced at its major scientific facilities, in use to manage the large volume of data assets.
- **Claddier (2005 - 07):** JISC funded project to investigate the data citation within Earth Observation data.
- **VizNet (2007-2010):** JISC network promoting the use of advance scientific visualisation.
- **ACRID (2010-11):** Publishing linked data for Earth Observation Data.
- **ISIC Visualisation (2010-11):** Design, commissioning and installation of a Hyperwall visualisation facility for the International Space Innovations Centre (ISIC).

## Research Interests

My current research area of expertise is in applying advanced computing research to develop infrastructure and techniques to efficiently manage scientific data, especially as it applies to large-scale scientific facilities. This includes:

- metadata modelling and representation for science data sets;
- ontology modelling for sharable models for science data sets;
- infrastructure services for data manipulation, data storage, data cataloguing, data sharing and data access;
- integrating data and computation services for modelling, analysis and analytics;
- preservation of software packages for reproducibility and reusability.
- workflow and data provenance of scientific processes;
- combining heterogeneous resources to provide a whole lifecycle view of science processes;
- long-term data preservation and reuse.

## Professional Activities

- Fellow of the British Computer Society since 2015 (member since 1998)
- I been external examiner for PhD theses, including at Cambridge and Cardiff.
- I have been a member of funding programme committees for JISC and BBSRC
- Reviewed papers for many journals and conferences.
- Member of the Oxford Brookes Industrial Liaison Committee
- Member of the steering committee for the SOFSEM international conference series

- Member of the editorial board for the international Journal of Open Research Software
- Co-Chair of the Research Data Alliance Interest Group on Research Data for Photon and Neutron Science.
- Deputy manager of the W3C Office for the UK and Ireland (2001-2010)

## Selected Publications

Brian is the author of over 150 publications, and invited presentations. For a complete list see: <http://epubs.stfc.ac.uk/search?st=browse-by-person&pid=6>

A selected list includes:

- PaNdata: Open Data Infrastructure for Photon and Neutron Sources  
J Bicarregui, B Matthews, F Schluenzen. Synchrotron Radiation News 28(2), 2015  
(doi:10.1080/08940886.2015.1013418)
- The Research Data Alliance Photon and Neutron Science Interest Group  
A Boehnlein, B Matthews, T Proffen, F Schluenzen. Synchrotron Radiation News 28(2), 2015  
(doi:10.1080/08940886.2015.1013421)
- Enabling Sharing and Reuse of Scientific Data  
S Dallmeier-Tiessen, R Darby, K Gitmans, S Lambert, B Matthews, S Mele, J Suhonen, M Wilson. New Review of Information Networking 19(1), 2014  
(doi:10.1080/13614576.2014.883936)
- Cloud computing in e-Science: research challenges and opportunities  
X Yang, D Wallom, S Waddington, J Wang, A Shaon, B Matthews, M Wilson, Y Guo, L Guo, JD Blower, et al. The Journal of Supercomputing 70(1), 2014 (doi:10.1007/s11227-014-1251-5)
- Experiences with a researcher-centric ELN  
KA Badiola, C Bird, WS Brocklesby, J Casson, RT Chapman, SJ Coles, JR Cronshaw, A Fisher, JG Frey, D Gloria, et al. Chemical Science 6(3), 2014 (doi:10.1039/c4sc02128b)
- Data authenticity and data value in policy-driven digital collections  
V Bunakov, C Jones, B Matthews, M Wilson  
OCLC Systems & Services: International digital library perspectives 30(4), 2014
- Data Management and Preservation Planning for Big Science  
Juan Bicarregui, N Gray, R Henderson, R Jones, Simon Lambert, Brian Matthews  
The International Journal of Digital Curation 8(1), 2013 (doi:10.2218/ijdc.v8i1.247)
- Opening Up Climate Research: A Linked Data Approach to Publishing Data Provenance  
A Shaon, S Callaghan, B Lawrence, B Matthews, T Osborn, C Harpham, A Woolf  
International Journal of Digital Curation 7(1), 2012 (doi:10.2218/ijdc.v7i1.223)
- Managing Risks in the Preservation of Research Data with Preservation Networks  
E Conway, BM Matthews, D Giaretta, SC Lambert, MD Wilson, N Draper. International Journal of Digital Curation 7(1), 2012
- Curating scientific research data for the long term : a preservation analysis method in context  
E Conway, D Giaretta, S Lambert, B Matthews. International Journal of Digital Curation 6(2), 2011
- Citation and peer review of data : moving towards formal data publication  
BN Lawrence, CM Jones, BM Matthews, SJ Pepler, SA Callaghan. International Journal of Digital Curation 6(2), 2011
- Enhancing the Core Scientific Metadata Model to Incorporate Derived Data  
E Yang, B Matthews, MD Wilson. Future Generation Computer Systems 29(2), 2013  
(doi:10.1016/j.future.2011.08.003)

- Using a core scientific metadata model in large-scale facilities. B Matthews, S Sufi, D Flannery, L Lerusse, T Griffin, M Gleaves, K Kleese/ International Journal of Digital Curation 5 (1), 106-118
- A Framework for Software Preservation  
Brian Matthews, Arif Shaon, Juan Bicarregui, Catherine Jones. International Journal of Digital Curation 5(1), 2010 (doi:10.2218/ijdc.v5i1.145)
- An evaluation of enhancing social tagging with a knowledge organization system. B Matthews, C Jones, B Puzon, J Moon, D Tudhope, K Golub, Marianne Lykke Nielsen. Aslib Proceedings 62 (4/5), 447-465 , 2010
- ICAT: Integrating data infrastructure for facilities based science. D Flannery, B Matthews, T Griffin, J Bicarregui, M Gleaves, L Lerusse, Roger Downing, Alun Ashton, Shoaib Sufi, Glen Drinkwater, Kerstin Kleese. e-Science'09. Fifth IEEE International Conference on e-Science, 201-207, 2009
- Virtual Organization Support within a Grid-Wide Operating System  
Massimo Coppola, Yvon Jégou, Brian Matthews, Christine Morin, Luis Pablo Prieto, Óscar David Sánchez, Erica Y Yang, Haiyan Yu. IEEE Internet Computing 12(2), 2008 (doi:10.1109/MIC.2008.47 )
- Enhancing social tagging with a knowledge organization system  
Koraljka Golub, Catherine Jones, Brian Matthews, Jim Moon, Marianne Lykke Nielsen, Douglas Tudhope. ALISS Quarterly (Association of Librarians and Information Professionals in the Social Sciences) 3(4), 2008. Presented at ALISS Summer Conference, 2008
- SKOS core: simple knowledge organisation for the web. A. Miles, B Matthews, M Wilson, D Brickley. International Conference on Dublin Core and Metadata Applications, pp. 3-10, 2005

## **DEBORAH ELLEN MIES**

### **Debbie Mies, US Industry Relations Manager, Granta Design, Ltd.**

Debbie Mies is one of the leading experts in materials information technology and its application to customer needs. A graduate of University of California, Irvine with background in chemistry and advanced composites, Debbie has specialized in Materials Information Technology for over twenty years. She has supported all aspects of the software development lifecycle from product specification to implementation, and actively participated in industry Standards initiatives concerned with materials information. Debbie has previously held positions in Product Management, Software Design, and Services at MSC Software. Debbie currently helps Granta customers in North America to develop the full potential of materials information technology in their engineering process.

#### **EXPERIENCE**

2013 - Present	<b>GRANTA DESIGN, LT.</b> , Cambridge, UK <b>Industry Relations Manager, US</b>
1994 - Present	<b>MSC.SOFTWARE CORPORATION</b> , Santa Ana, CA <b>Senior Product Manager and Designer</b>
2009 - Present	<b>Senior Project Manager, Consulting Services</b>
2006 - 2008	<b>Senior Implementation Specialist</b>
1997 - 2005	<b>Mvision Databank Product Manager</b>
1994 - 1997	
1989 - 1994	<b>PDA ENGINEERING</b> , Costa Mesa, CA <b>Polymer Chemist</b>

#### **EDUCATION**

**University of California Extension, Irvine, CA**

Product Management, Project Management, Data Warehousing

**California State University, Long Beach, CA**

M.A. Candidate in Industrial Technology/ Plastics Technology

**University of California, Irvine, CA**

Graduate Courses in Polymer Chemistry

**University of California, Irvine, CA**

B.S. Chemistry, Minor Biology

#### **TECHNICAL TRAINING**

Pro/Engineer CAD / CAM Training

Mvision Materials Data Management Software

UNIX, Windows, Linux operating Systems

Oracle, Microsoft Access Databases

Microsoft Products  
HTML, XML, JavaScript Programming

**ASSOCIATIONS**

Society of Plastics Engineers – Board Member 1994  
American Chemical Society  
ASM International Materials Property Database Committee Chair  
(2009-2010)  
TMS ICME Committee

**STANDARDS ORGANIZATIONS** (Active Participant)

CEN-ESSL (initiative to standardize the interchange of materials test data)  
MatML Coordination Committee  
Mil-HDBK 5 Schema Development Committee member  
Mil-HDBK 17 Schema Development Committee  
STEP/PDES

**PUBLICATIONS**

*Thermoreactive Aircraft Coatings (TRAC) Program*  
Kurt E. Jechel, Deborah E. Bielecka, PDA Engineering, 01 March 1995

*Building Mvision Databanks*  
Deborah E. Bielecka, MSC.Software Corporation, 1997

*Handbook of Material Selection*  
Myer Kutz Editor, Deborah Mies contributing author, John Wiley and Sons, 2002

## Yibin Xu

### ● PROFESSIONAL PREPARATION

Dr. Information Sc. Information process, Nagoya University (2007)

M. Information Sc. Information process, Nagoya University (2000)

Dr. Eng. Inorganic material science, Shanghai Institute of Ceramics,  
Chinese Academy of Sciences (1994)

B. Sc. Theoretical physics, Nanjing University (1988)

### ● POSTDOCTORAL APPOINTMENTS

National Industrial Research Institute of Nagoya, 1995-1997

### ● APPOINTMENTS

Apr. 2014-date Group leader, Database Group, Materials Information  
Station, National Institute for Materials Science

Apr. 2007-Mar. 2014 Principal Researcher, National Institute for Materials Science

Apr. 2005-Mar. 2007 Senior Researcher, National Institute for Materials Science

Apr. 2002-Mar. 2005 Researcher, National Institute for Materials Science

Apr. 2000-Mar. 2002 System Engineer, CTI Co., Ltd.

Apr. 1994-Jan. 1995 Associate Research Fellow  
Shanghai Institute of Ceramics, Chinese Academy of  
Sciences.

### ● PUBLICATIONS

#### *Five most relevant publications for proposal*

1. Inorganic Materials Database for Exploring the Nature of Material, Y. Xu, M. Yamazaki, P. Villars, Jpn. J. Appl. Phys, 50, 11RH02 (2011)
2. Interfacial Thermal Conductance Database, Y. Xu, Kinzoku, Materials Science & Technology, 81 (12), 69, (2011)
3. Prediction of Thermal Conductivity of Composite Materials, Y. Xu, Y. Tanaka, H. Guo, M. Yamazaki, J. Power and Energy System, 2(3), 1048 (2008)
4. Computation of Interfacial Thermal Resistance by Phonon Diffuse Mismatch Model, H. Wang, Y. Xu, M. Shimono, Y. Tanaka, M. Yamazaki, Materials Transactions, 48(9), 2349 (2007)
5. Prediction and Relation of Thermal Conductivity with Average Relative Atomic Mass and Density for Semiconducting Compound Functional Crystal Materials, Q. Wu, Y. Xu, T. Xi, Jpn. J. Appl. Phys. 46(6A), 1441 (2007)

#### *Five other publications*

1. Phonons with long mean free paths in a-Si and a-Ge, T. Zhan, Y. Xu, M. Goto, Y. Tanaka, R. Kato, M. Sasaki, Y. Kagawa, Appl. Phys. Lett. 104, 071911 (2014)
2. Thermal conductivity of sputtered amorphous Ge films, T. Zhan, Y. Xu, M. Goto, Y. Tanaka, R. Kato, M. Sasaki, Y. Kagawa, AIP Advance, 4, 027126 (2014)
3. Three-dimensional strutted graphene grown by substrate-free sugar blowing for high-power-density supercapacitors, W. Wang, Y. Zhang, C. Zhi,



- X. Wang, D. Tang, Y. Xu, Q. Weng, X. Jiang, M. Mitome, D. Golberg, Y. Bando, Nature Communications, 4:2905, DOI:10.1038/ncomms3905
4. Thermal conductivity of ZnO thin film produced by reactive sputtering, Y. Xu, M. Goto, R. Kato, Y. Tanaka, Y. Kagawa, J. Appl. Phys. 111, 084320 (2012)
  5. Highly Thermo-conductive Fluid with Boron Nitride Nanofillers, C. Zhi, Y. Xu, Y. Bando, D. Golberg, ACSNANP 5(8), 6571 (2011).

● SYNERGISTIC ACTIVITIES

Awards:

1. Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology, 2012
2. NIMS President Award, 2012
3. Orga-Techno Award, 2007
4. Since and Technology Agency Fellowship, 1995
5. Inst. for Transfer of Industrial Technology Fellowship, 1996
6. Chinese Science and Technology Prize for Youth, ( the Organization Department of the Central Committee of the Communist Party of China, the Ministry of Personnel Affair of China & the Science Society of China), 1994
7. Science and Technology Prize for Youth. (the Chinese Silicate Society), 1994
8. The Prize for Progression of Science and Technology, Grade A, (the Chinese Academy of Sciences), 1993

Director:

1. Member: Asian Materials Data & Database Committee
2. Member: World Research Institute Forum
3. Member: Eco-Material Forum Publication Committee
4. Member: JSMS Committee on Fatigue Database

Member executive committee:

1. IUMRS-ICA2014, Symposium A-1 Analytical and Assessment Methods in Materials and Environmental Technologies, Aug. 24-30, 2014, Fukuoka, Japan
2. 3<sup>rd</sup> Asian Materials Database Symposium, Apr. 15-18, 2012, Naha, Japan
3. 2<sup>nd</sup> Asian Materials Database Symposium, Mar. 10-14, 2010, Sanya, China
4. 1<sup>st</sup> Asian Materials Database Symposium, Jan. 29-Feb. 3, Jeju, Korea
5. International Symposium on Materials Database 2008, Jul. 17-18, 2008, Tsukuba, Japan
6. International Symposium on Materials Database 2007, Mar. 16, 2007, Tsukuba, Japan
7. International Symposium on Materials Database 2006, Jan. 20, 2006, Tokyo, Japan
8. International Symposium on Materials Database 2005, Mar. 15, 2005, Tokyo, Japan

● COLLABORATORS & OTHER AFFILIATIONS

Advisor:

1. Internship Ph.D. student, Hu Anqi, Department of Mechanical Engineering, Northwestern University. Advisor: Professor L. Cate Brinson (2015)
2. Internship Ph.D. student, He Zhao, Department of Mechanical Engineering, Northwestern University. Advisor: Professor L. Cate Brinson (2014)

## Curriculum Vitae

Name: Haiqing YIN

Date of Birth: April, 1971

Nationality: P.R.China



### Education

- Ph.D., Material Science and Engineering, University of Science and Technology Beijing, Beijing, China, 2008.
- M.S., Corrosion and protection of Metals and alloys, Xi'an Jiaotong University, Xi'an, China, 1996.
- B.S., Metal materials and heat treatment, Xi'an Jiaotong University, Xi'an, China, 1993.

### Work Experience

- **University of Science and Technology Beijing**, China, 2002- Present, Professor of Materials Data and Powder metallurgy.
- **Pennsylvania State University**, USA, 2011/04 – 2011/10, Guest Professor in CISP of Mechanical Engineering Department.
- **Osaka University**, Osaka, Japan, 2000/09-2002/05, Visiting researcher.
- **Beijing University of Chemical Technology**, China, 1996/08- 2000/08, Lecturer.

### Professional Activities

- **Board member**, Asia Materials Data Committee (AMDC) and Contact person of AMDC in China, 2010-present
- **Deputy Director**, Beijing Key Laboratory for Materials Genome Engineering, 2015-present
- **Key researcher**, National Project of “China Materials Scientific Data Sharing Network”, 2006-present
- **Organizing committee member**, Scientific Data congress in China, and **Organizer** of session “Materials data & application”, 2014-2015
- **Editorial Board Member**, Journal “Powder Metallurgy Industry” in China, 2012-present
- **Drafter**, Materials Data part of Consulting Reports ( submitted to the State Department from Chinese Academy of Sciences and Chinese Academy of Engineering) , 2013-2014

### Publication

1. Yin Haiqing, Liu Guoquan, Jiang Xue, Zhang Ruijie, Qu Xuanhui. Materials databases and constructing national public service platform of materials data. Science & Technology Review (in Chinese), 2015, 33(10):50-59

2. Yin Haiqing, Zhang Ruijie, Liu Guoquan, Qu Xuanhui, Xie Jianxin. Development of the Materials Databases. *Journal of Chinese Ceramic Society*, 2014,1(1):48-52
3. He Li , Haiqing Yin, Dil Faraz Khan, Huiqin Cao, Zainul Abideen, Xuanhui Qu. High velocity compaction of 0.9Al<sub>2</sub>O<sub>3</sub>/Cu composite powder. *Materials and Design* , 2014,57: 546-550
4. Dil Faraz Khan, Haiqing Yin, He Li, Zainul Abideen, Asadullah, Xuanhui Qu, Mujtaba Ellahi. Effect of impact force on Ti-10Mo alloy powder compaction by high velocity compaction technique. *Materials and Design*, 2014,54: 149-153
5. Yi S J, Yin H Q, Zheng J, Khan D F, Qu X H. The first-principles study on the mechanical and electronic properties about rim phase and hard phase of Ti(C,N) based cermets. *Computational Material Science*, 2013, 79: 417-423.
6. Yi S J, Yin H Q, Chen K, Khan D F, Zheng Q J, Qu X H. Research on microstructure and properties of the nano-TiN modified Ti(C,N)-based cermets fabricated by powder injection molding and die pressing. *International Journal of Minerals, Metallurgy and Materials*, 2013, 20(11): 1115-1121.
7. Khan DF, Yin HQ, Li H, Qu XH, Khan M, Ali S, Iqbal MZ. Compaction of Ti-6Al-4V powder using high velocity compaction technique, *MATERIALS & DESIGN*, 2013, 50: 479-483.
8. Khan DF, Yin HQ, Usman Z, Khav M, Yuan XJ, Wang WH, Qu XH. Improvement of a High Velocity Compaction Technique for Iron Powder, *ACTA METALLURGICA SINICA-ENGLISH LETTERS*, 2013,26(4): 399-403.
9. Khan DF, Yin HQ, Khan M, Asa dullah, Qu XH. Analysis of Density and Mechanical Properties of Iron Powder with Upper Relaxation Assist through High Velocity Compaction, *MATERIALS PERFORMANCE, MODELING AND SIMULATION*, 2013, 749: 41-46.
10. Xin-lei Ni, Hai-qing Yin, Lin Liu, Shan-jie Yi, and Xuan-hui Qu. Injection molding and debinding of micro gears fabricated by micro powder injection molding, *International Journal of Minerals, Metallurgy and Materials*, 2013,20(1): 1-6.
11. Haiqing Yin, Guoquan Liu, Ruijie Zhang, Xuanhui Qu. Construction of Material Database Infrastructure for Materials Genome Initiative, *IUMRS-ICAM2013*,2013-0,Qingdao, China
12. Haiqing Yin, Jia Guan, Xianjie Yuan, Dil Faraz Khan, Xuanhui Qu. Study on High-strength Aluminum Alloy 7050 Powder formed by High Velocity Compaction, The 2nd International Conference on Powder Metallurgy in Asia, 2013-11,Xiamen, China.
13. Haiqing Yin, Guoquan Liu, Xuanhui Qu. From the Powder Metallurgy Data To the Sustainable Development of Materials Database, *The 3rd Asian Materials Data Symposium*, 2012.04.13-16, Noha, Japan.
14. Xian-jie Yuan, Hai-qing Yin, Rafi-ud Din, Khan D.-F, Xuan-hui Qu. Study on the impact force and green properties of high-velocity compacted aluminum alloy

powder, International Journal of Minerals, Metallurgy and Materials,  
2012,19(12): 1107-1113.