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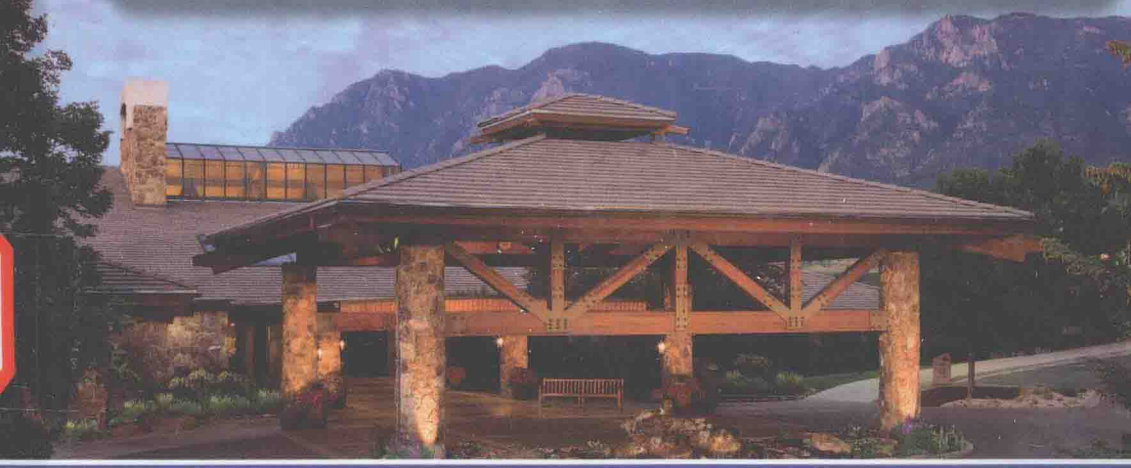
Proceedings of the 3rd World Congress on Integrated Computational Materials Engineering (ICME 2015)

May 31–June 4, 2015 • Cheyenne Mountain Resort
Colorado Springs, Colorado, USA

EDITORS:

Warren Poole • Steve Christensen • Surya Kalidindi
Alan Luo • Jonathan Madison • Dierk Raabe • Xin Sun



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3rd World Congress
on Integrated Computational Materials Engineering (ICME 2015)

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TMS (The Minerals, Metals & Materials Society)

Held

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Preface

This is a collection of manuscripts presented at the 3rd World Congress on Integrated Computational Materials Engineering, a specialty conference organized by The Minerals, Metals & Materials Society (TMS) and the seven congress organizers, and held in Colorado Springs, Colorado, USA, on May 31 to June 4, 2015.

Integrated Computational Materials Engineering (ICME) has received international attention and has been proven to shorten product and process development time, while lowering cost and improving outcome. Building on the great success of the first two World Congresses on Integrated Computational Materials Engineering, the 3rd World Congress on ICME convened researchers, educators, and engineers to assess the state-of-the-art ICME and determine paths to further the global advancement of ICME. Over 150 authors and attendees from all over the world contributed to this congress in the form of presentations, lively discussions, and manuscripts presented in this volume. The international advisory committee members representing 10 different countries actively participated and promoted the congress.

The specific topics highlighted during this congress included: ICME Success Stories and Applications with separate sessions on Lightweighting, Composites, Ferrous, and Non-ferrous Applications, ICME Infrastructure and Tools, Modelling at Different Length Scales, Process and Performance Modelling, ICME Implementation and Case Studies. The congress consisted of both plenary sessions and parallel sessions with 20 invited presentations from international experts and a special panel discussion. From the evening poster sessions, outstanding posters were selected for awards, which were presented to the authors at the congress dinner. The congress ended with a closing panel of experts focusing the discussion on the needed next steps forward to help ensure a boarder and more global implementation of ICME in the future.

The 42 papers presented in these proceedings represent a cross section of the presentations and discussions from this congress. It is our hope that the 3rd World Congress on ICME and these proceedings will further the global implementation of ICME, broaden the variety of applications to which ICME is applied, and ultimately help industry design and produce new materials more efficiently and effectively.

Acknowledgments

The organizers/editors would like to acknowledge the contributions of a number of people without whom this 3rd World Congress, and the proceedings, would not have been possible.

First, we would like to offer many thanks to the TMS staff who worked tirelessly to make this an outstanding congress and excellent proceedings.

Second, we want to thank the international advisory committee for their input in the planning, the promotion and their participation in the congress. This international committee included:

John Ågren, *KTH - Royal Institute of Technology, Sweden*
John Allison, *University of Michigan, USA*
Dipankar Banerjee, *Indian Institute of Technology, India*
Dennis Dimiduk, *U.S. Air Force Research Laboratory, USA*
Mathew Halls, *Schrodinger, USA*
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Alejandro Strachan, *Purdue University, USA*
Anthony Waas, *University of Michigan, USA*
James Warren, *National Institute of Standards and Technology, USA*

Finally, we would especially like to acknowledge the financial support of all our sponsors. We are also grateful for the participation and contributions of all of the attendees.

Conference Editors/Organizers

Warren Poole is the Head of the Department of Materials Engineering at The University of British Columbia and holds the Rio Tinto Alcan Chair in Materials Process Engineering. He received his Ph.D. from McMaster University which was followed by a NSERC Post-Doctoral Fellowship at the University of Cambridge, UK. Professor Poole has published over 150 journal and conference papers related to the deformation, fracture and microstructure evolution in light alloys and steels. He works closely with leading industrial companies in the world to transfer the knowledge gained from his research to industrial receptors. In addition, he serves on the international scientific committee for the two major conferences on light metals and is on the advisory board of LATEST 2 research program at the University of Manchester. He has won numerous best paper and poster awards, the 2013 Canadian Metal Physics Award, the 2014 Award of Excellence from the International Magnesium Association, a Killam Research Fellowship, given over 50 invited talks and was a recipient of the Alan Blizzard Award for excellence in teaching. Professor Poole was the Scientific Director of the NSERC Strategic Research Network (MagNET) from 2008 to 2014.

Steve Christensen worked for Boeing for nearly 40 years. Assignments have included materials development for the B-1, 757, 767, Advanced Tactical Fighter (now F-22), numerous special projects and the Joint Strike Fighter. Research emphasis since the mid-1990s has been on the development of a deformation based understanding of composite constituent materials performance known as Onset Theory with emphasis on improving polymer distortional deformation as the key to increased composite performance. Over the past 12 years the theory in conjunction with computational simulations has been used to develop improved matrix materials for composites. Many simulation techniques specific to thermoset polymers have also been developed in order to understand the structure-property relationships of polymer matrix materials, polymer-fluid interactions, chemical reactivity and environmental resistance all with the aim of developing composite matrix chemistries that exploit the teachings of onset theory.

Surya R. Kalidindi earned a B.Tech. in Civil Engineering from the Indian Institute of Technology, Madras, an M.S. in Civil Engineering from Case Western Reserve University, and a Ph.D. in Mechanical Engineering from the Massachusetts Institute of Technology. After his graduation from MIT in 1992, Surya joined the Department of Materials Science and Engineering at Drexel University as an Assistant Professor, where he served as the Department Head during 2000-2008. In 2013, Surya accepted a new position as a Professor of Mechanical Engineering in the George W. Woodruff School at Georgia Institute of Technology, with joint appointments in the School of Computational Science and Engineering and in the School of Materials Science and Engineering. Surya's research efforts over the past two decades have made seminal contributions to the fields of crystal plasticity, microstructure design, spherical nanoindentation, and materials informatics. His work has already produced about 200 journal articles, four book chapters, and a new book on Microstructure Sensitive Design. His work is well cited by peer researchers as reflected by an h-index of 50 and current citation rate of about 1000 citations/year (Google Scholar). He has recently been awarded the Alexander von Humboldt award in recognition of his lifetime achievements in research. He has been elected a Fellow of ASME, ASM International, and TMS. He is also a member of the inaugural class of TMS MGI Ambassadors.

Alan Luo is Professor of Materials Science and Engineering and Professor of Integrated Systems Engineering (Manufacturing) at The Ohio State University (OSU) in Columbus, OH, USA. Prof. Luo is also Director of OSU Light Metals and Manufacturing Research Laboratory (LMMRL). Prior to joining OSU in July 2013, Dr. Luo was a GM Technical Fellow at General Motors Global Research and Development Center (Warren, MI, USA) with 20 years of industrial experience. Prof. Luo is an elected Fellow of ASM (American Society of Metals) International and SAE (Society for Automotive Engineers) International. He has 17 patents and more than 180 technical publications in advanced materials, manufacturing and applications. Dr. Luo won two John M. Campbell Awards for his fundamental research, and three Charles L. McCuen Awards for research applications at GM. He received the TMS (The Minerals, Metals & Materials Society) Brimacombe Medalist Award and SAE Forest R. McFarland Award in 2013, USCAR (United States Council for Automotive Research) Special Recognition Award in 2009, and ASM Materials Science Research Silver Medal in 2008. Dr. Luo's research is also recognized by several Best Paper awards from TMS, SAE and AFS (American Foundry Society). Prof. Luo is presently Chair of SAE Materials Engineering Activity and Vice Chair of TMS Light Metals Division.

Jonathan D. Madison, Ph.D. is a Senior Member of Technical Staff at Sandia National Laboratories in Albuquerque, New Mexico within the Materials and Mechanics Department. Madison received his Bachelor's degree from Clark Atlanta University in Engineering Science with a concentration in Mechanical Engineering and his M.S. and Ph.D. in Materials Science and Engineering from the University of Michigan in 2007 and 2010 respectively. Throughout his academic matriculation, Dr. Madison has supported basic and applied research at Washington State University, Pullman, WA; the Naval Research Laboratory, Washington, D.C.; and the Massachusetts Institute of Technology in Cambridge, Massachusetts. He maintains active membership in The Association for Iron & Steel Technology (AIST), ASM International (ASM), The American Society of Mechanical Engineers (ASME) and The Minerals, Metals & Materials Society (TMS). His research interests focus on the intersection of experimental and computational techniques for three-dimensional reconstructions of microstructure, their quantitative characterization and accompanying models of microstructural evolution. The department he currently serves provides advanced multi-scale characterization to adapt materials-based insight and solutions to modern engineering problems. Dr. Madison has to his credit 9 peer-reviewed journal articles, 4 Department of Energy published technical reports and over 35 national and international technical presentations including 9 invited talks.

Dierk Raabe graduated from RWTH Aachen in physical metallurgy and metal physics. Later he joined Carnegie Mellon University and the High Magnet Field Laboratory in Tallahassee. Currently he is Chief Executive of the Max-Planck Institut für Eisenforschung in Düsseldorf and Professor at RWTH Aachen University. His research interests are in microstructures, simulations and mechanical properties of metallic alloys. He wrote and edited several books on these topics, such as Computational Materials Science (1998), Continuum Scale Simulation of Engineering Materials (2005), and Crystal Plasticity FEM in Materials Science and Engineering (2010) as well as more than 450 peer reviewed publications. Raabe places emphasis on comparing simulations with experiments conducted under complex boundary conditions. He uses quantum mechanical simulations for engineering materials design and property predictions and combines atomistic simulations with atomic scale characterization. The common vision in these activities lies in using predictive simulations and their consequent engineering application for inventing advanced alloys. In 2004 Raabe received the highest German research award (Leibniz-Award). 2008 he was awarded the Lee Hsun Lecture Award of the Chinese Academy of Sciences

and in 2011 the Weinberg Lecture Award of the University of British Columbia. In 2012 he received an ERC advanced grant and in 2014 became Honorary Professor at the Katholieke Universiteit Leuven. Since 2010 he is a member of the German Council of Science and Humanities. Since 2012 he is the chairman of the Governors Board of RWTH Aachen University. He is a member of the German National Academy Leopoldina.

Xin Sun is a Laboratory Fellow and the Technical Group Leader for the Computational Engineering Group at Pacific Northwest National Laboratory in Richland, Washington. She got her B.S.E from Shanghai Jiao Tong University, M.S.E and Ph.D. from the University of Michigan, Ann Arbor, MI. Dr. Sun has a broad range of experience in the areas of applied mechanics and computational materials. Her expertise lies in applying and developing the multi-scale and multi-physics modeling tools in solving practical engineering problems associated with advanced multiphase lightweight materials and thermal-mechanical manufacturing processes.

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ICME Applications

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TMS (The Minerals, Metals & Materials Society), 2015

IMPORTANCE OF CONTROLLING MICROSTRUCTURE HETEROGENEITY WHEN DESIGNING STEEL

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Keywords: Heterogeneity, Recrystallization, Phase transformation, Hydrogen embrittlement

Abstract

Steel has been used since long in the past, but there still remain many unexplored possibilities. In order to draw out this latent potential, the concept of materials integration is garnering attention in view of discontinuously improving the function and performance of steel products, while reducing the necessary development period. In this paper, considering the utilization of materials integration, the evolution of the microstructure during plastic deformation and phase transformation as well as controlling hydrogen embrittlement are discussed in terms of heterogeneity. In addition, a brief outlook on the future of materials integration is presented.

Introduction

One characteristics of steels is that they have a very wide range of strength, varying by up to about 100 times, as shown in Fig. 1 [1]. However, the strength levels used practically in various markets are only a fraction of steel's potential [1]. In this sense, steel can be called an attractive material which still has many unexplored possibilities. However, there remain many technical issues to be solved in order to draw out this latent potential.

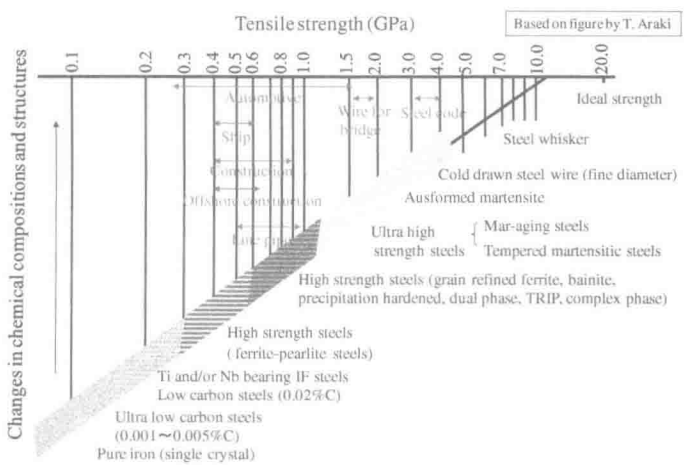

Fig. 1 Spectrum of steel strengths together with the strength levels of practically used steels [1].

Integrated Computational Materials Engineering (ICME) is an important concept and is considered to be the future direction of development.