TMS ICME

MANUFACTURING

DESIGN MATERIALS

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

TMS

Springer


TMS
ICME
MANUFACTURING
DESIGN
MATERIALS

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

Sponsored by

TMS (The Minerals, Metals & Materials Society)

Held

May 31–June 4, 2015

Cheyenne Mountain Resort

Colorado Springs, Colorado, USA

Edited by

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

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

ISBN 978-3-319-48612-3 ISBN 978-3-319-48170-8 (eBook)
DOI 10.1007/978-3-319-48170-8

Chemistry and Materials Science: Professional

Published by Springer International Publishers, Switzerland, 2016
Reprint of the original edition published by John Wiley & Sons, Inc., 2015, 978-1-119-13949-2

Printed on acid-free paper

This Springer imprint is published by Springer Nature
The registered company is Springer International Publishing AG
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

TABLE OF CONTENTS

3rd World Congress on Integrated Computational Materials Engineering

ICME Applications

ICME Building Blocks

ICME Success Stories and Applications

Integration of ICME Building Blocks: Multi-Scale Modeling

Modeling, Data and Infrastructure Tools

Process Optimization

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*

Juergen Hirsch, *Hydro Aluminum, Germany*

Dorte Juul Jensen, *Risoe National Laboratory, Denmark*

Nack Kim, *Pohang University of Science and Technology, Korea*

Peter Lee, *Imperial College, UK*

Mei Li, *Ford Motor Company, USA*

Baicheng Liu, *Tsinghua University, China*

Jiang-Feng Nie, *Monash University, Australia*

Tresa Pollock, *University of California Santa Barbara, USA*

Anoush Poursartip, *University of British Columbia, Canada*

Gary Purdy, *McMaster University, Canada*

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.

3rd World Congress

on Integrated Computational Materials Engineering (ICME 2015)

ICME Applications

3rd World Congress on Integrated Computational Materials Engineering (ICME 2015)
Edited by: Warren Poole, Steve Christensen, Surya R. Kalidindi, Alan Luo, Jonathan D. Madison, Dierk Raabe, and Xin Sun
TMS (The Minerals, Metals & Materials Society), 2015

IMPORTANCE OF CONTROLLING MICROSTRUCTURE HETEROGENEITY WHEN DESIGNING STEEL

Kohsaku Ushioda[1], Hideaki Sawada[1], Masaaki Sugiyama[1]

[1]Nippon Steel & Sumitomo Metal Corp., 20-1 Shintomi, Futtsu, Chiba, 293-8511, Japan

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.

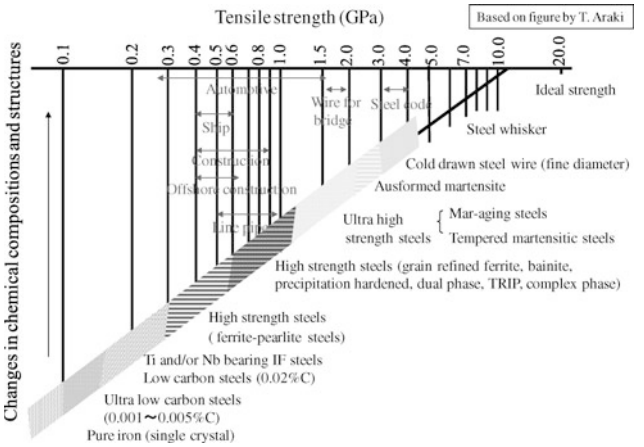


Fig. 1 Spectrum of steel strengths together with the strength levels of practically used steels [1].

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

In this paper, focus is first placed on the heterogeneous deformation structure in poly crystal Fe. Then, the effect of Boron (B) addition on retarding the austenite (γ) to ferrite (α) phase transformation is discussed. Also, since hydrogen embrittlement is one of the prohibiting factors to further increases in strength, the mechanism by which precipitates trap hydrogen is presented. Finally, the future outlook of ICME is presented.

Heterogeneous deformation structure and recrystallization

Heterogeneous deformation structure becomes most essential when controlling the microstructure and crystal orientation by recrystallization and phase transformation. The structure formed by rolling is heterogeneous as schematically illustrated in Fig. 2 [2]. The grain boundary region, shear band and deformation zone around hard second particles are typical heterogeneous deformation structures.

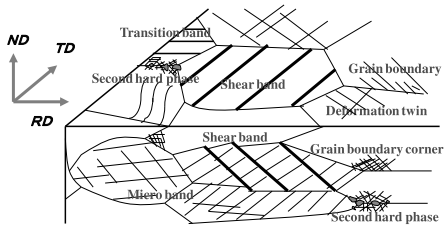


Fig. 2 Schematic illustration of the heterogeneity of a cold-rolled structure [2].

An example of heterogeneous deformation nearby a grain boundary is shown in Fig. 3 [3]. IF (Interstitial Free) steel with a grain diameter of about 40μm was cold-rolled by 80%. As a result of the statistical analysis of 84 grain boundaries parallel to the rolling plane, the boundaries were classified into one of the following three boundaries depending on the neighboring orientation relationship; a) relatively flat boundary, b) irregularly serrated boundary, and c) boundary associated with fine grains. In particular, it is worthy to note that 22 of the 84 boundaries analyzed were classified as case c).

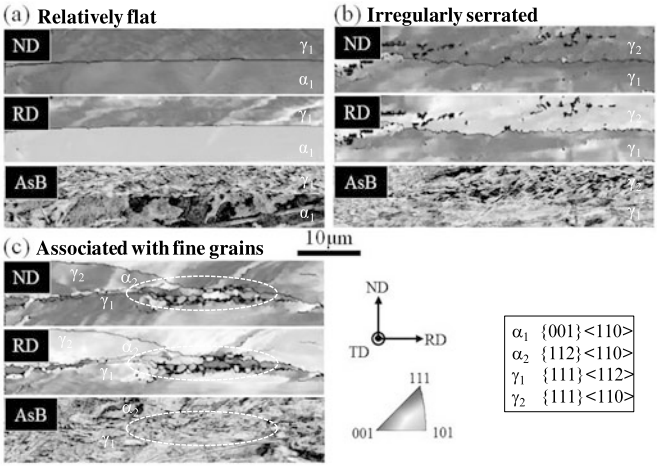


Fig. 3 Heterogeneous cold-rolled microstructure in the vicinity of a grain boundary [3].

A TEM micrograph of a shear band and its 3D schematic illustration is shown in Fig. 4 [3, 4]. Fe-0.02C (mass%) was water quenched from 700ºC and then cold-rolled by 70%. Intensive shear was localized in the shear band, and the crystal rotated from {111}<112> in the matrix to Goss orientation ({110}<001>) in the shear band around the TD//<110> axis.

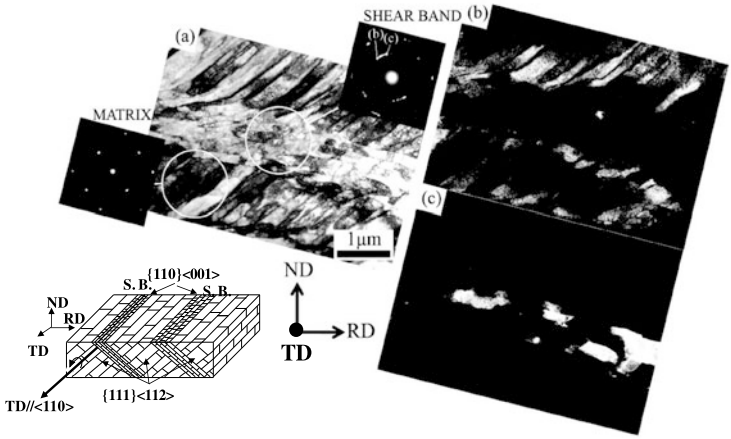


Fig. 4 TEM bright field image showing shear band, and diffraction pattern together with dark field images. 3D schematic illustration of shear band is also presented. [3, 4]

The heterogeneous deformation around the hard second phase is shown in Fig. 5 [5]. Fe-0.07C-16Cr was quenched from two phase region and then cold-rolled by 75%. EBSD analysis shows that large strain was concentrated around the hard α' (Fig. 5 a). However, when α' was tempered at 550 ºC for 1h prior to cold-rolling, the deformation became rather uniform (Fig. 5b).

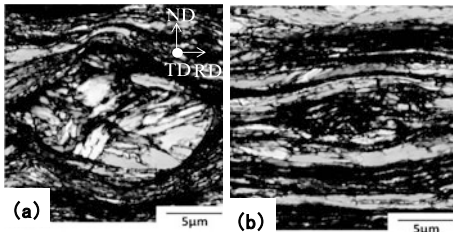


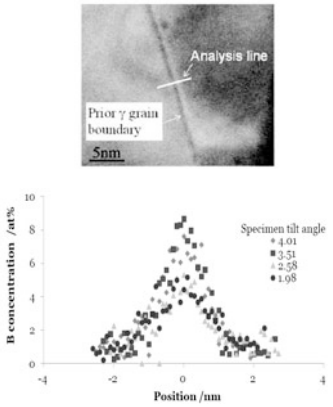
Fig. 5 Deformation zone around a hard second phase in Fe-0.07C-16Cr. (a) quenched α' and (b) tempered α' [5].

The heterogeneity in deformations has neither been systematized experimentally nor been rigorously predicted. Therefore, there is a strong need to predict the heterogeneity by 3D CP-FEM or FFT and then verify the predictions by, for example, 3D XRD experiments. Ultimately, a numerical approach is expected to predict the evolution of the microstructure and texture during recrystallization and phase transformation using predicted heterogeneous deformation structure through a combination of the crystal plasticity and phase field method. Despite the fact that research is being carried out in this direction [6-8], there still exist issues to be overcome in the future.

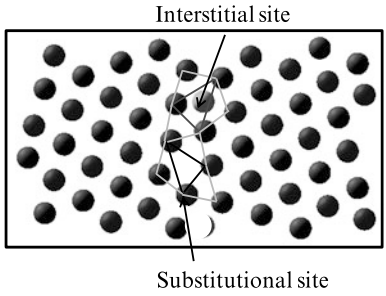
B segregation to the γ grain boundary and its effect on the γ/α phase transformation

It is well known that the addition of several massppm of B retards the γ/α phase transformation and subsequently improves hardenability, because B segregates to the prior γ grain boundary. Therefore, the addition of a small amount of B is effective from the standpoint of reducing the amount of necessary alloying elements and relaxing the process conditions.

Recently, B segregation to the γ boundary has been investigated using CS-STEM [9]. B segregates as much as 1600 times with a thickness of about two atomic layers (Fig. 6 a). On the other hand, the first principle calculation was applied to B segregation. The segregation energy to the Σ9 boundary, which is rather close to the general boundary, was evaluated [10]. Taking into



a)



b)

Fig. 6 a) STEM image and B concentration profiles measured by CS-STEM with several tilt angles around the prior γ grain boundary of Fe-0.05C-1.5Mn-3Ni-0.0011B (mass %) annealed at 950ºC for 60s, then cooled to 650ºC with a cooling rate of 30ºC/s followed by He quenching [9], and b) schematic view of B segregation into Σ9 grain boundary and structure units after first principle calculation [10].

consideration structure relaxation, magnetism and change in lattice constant at high temperature, the segregation energy varied from -2.24 to -0.70 eV, which is similar to the value -0.59~-1.0 eV found by Auger spectroscopy. Moreover, a calculated grain boundary structure unit as shown in Fig. 6 b) resembled the one observed in the Σ9 Cu grain boundary [10].

The kinetic model for γ/α phase transformation was studied taking into account B segregation to the γ boundary using the difference in grain boundary energy $\Delta\gamma^{\gamma\gamma}$ described in Eq. (1) [11]:

$$\Delta\gamma^{\gamma\gamma} \fallingdotseq -\delta / (V_m^{gb}) RTkx^{\gamma} \qquad (1)$$

, where, δ, V_m^{gb}, k *and* x^{γ} are the thickness, molar volume, segregation coefficient and concentration of B at the γ grain boundary, respectively.

A value of -0.12Jm^{-2} for $\Delta\gamma^{\gamma\gamma}$ was obtained by substituting experimentally determined values. Fig. 7 shows the relationship between the critical activation energy for α nucleation at the 4-grain junction at 705 ºC under conditions where the γ/α interface energy was 0.5Jm^{-2} and 0.6Jm^{-2}. It is clear that α nucleation is drastically retarded due to the fact that the addition of 0.002% B decreases $\gamma^{\gamma\gamma}$ by 0.12Jm^{-2}. Furthermore, DICTRA calculations suggest that the addition of B does not affect the α growth, which is in good agreement with the experimental result [11]. The coexistent strong effect of Nb and Mo with B on γ/α phase transformation is well known; however, the effect

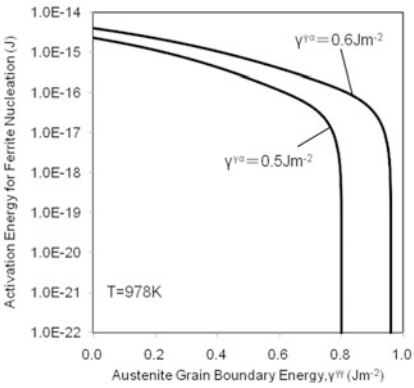


Fig. 7 Calculated activation energy for α nucleation as a function of γ grain boundary energy $\gamma^{\gamma\gamma}$ at 705ºC for two γ/α interfacial energies $\gamma^{\gamma\alpha}$ [11].

needs to be modeled in order to more effectively exploit the addition of B.

Resistance to hydrogen embrittlement by means of hydrogen trap

Hydrogen embrittlement is one of the inhibiting factors to further strengthening steel. Irrespective of the various mechanisms proposed for hydrogen embrittlement, it is essential to trap hydrogen by fine precipitates. The TiC/α-Fe interface is an example of trap site. A direct observation of the trap site was successfully made by 3D AP as shown in Fig.8 [12]. The material used was precipitation hardened steel of 0.03C-0.2Mn-3.0Al-0.1Ti, which was water-quenched from 1250 ºC in α-Fe phase followed by aging at 580 ºC for 4h in order to form fine TiC. AP observation was carried out after charging deuterium into the specimen. The reason for using deuterium was to improve the detection sensitivity, because deuterium occurs very infrequently in nature, but has chemical characteristics similar to hydrogen. The trapping of deuterium in the TiC/Fe interface is clearly shown in Fig.8, which is presumably due to elastic strain and/or misfit dislocation in the semi-coherent interface.

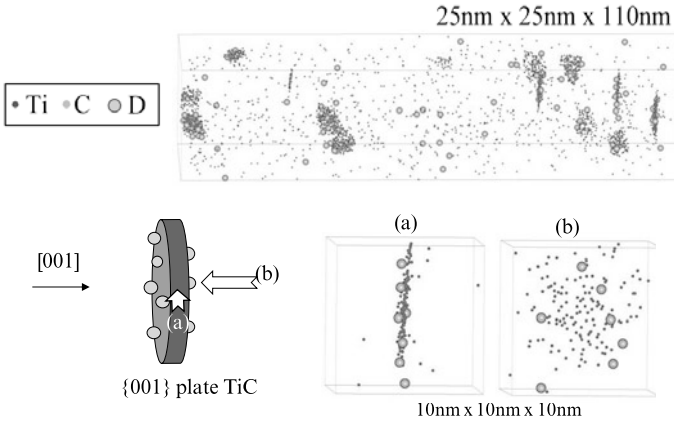


Fig. 8 3D AP elemental mapping showing deuterium trapped by TiC in α-Fe [12].

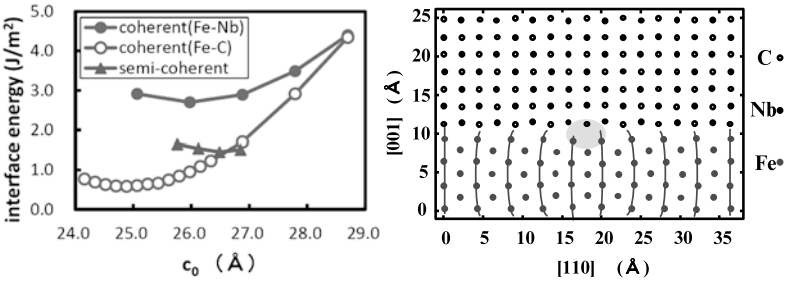
Recently, the interfacial energy of NbC/α-Fe has been predicted by first principle calculation through the application of the order (N) method [13]. Fig.9 a) shows the results of the interfacial energy for coherent and semi-coherent interfaces. The lowest interfacial energy, 0.6J/m^2, occurred at the coherent interface, where the C atom of NbC positions on an Fe atom in the matrix. On the contrary, the interfacial energy at the semi-coherent interface was as large as 1.2J/m^2. The atomic configuration of semi-coherent interfaces is illustrated in Fig.9 b), where the lattice in the matrix bends in such a manner for an Fe atom to site beneath the C atom of NbC resulting in the formation of a misfit dislocation.

Nano-precipitates of the alloy carbides TiC, NbC and VC have been characterized as having the hydrogen trapping property [14]. The hydrogen trapping ability of (semi-) coherent alloy carbides was clarified to vary in the descending order of NbC > TiC >> VC presumably due to the difference in lattice misfit. The hydrogen trap energy depending on the trap site may be obtained by

Table1 Calculated trap energy (kJ/mol) of a hydrogen atom by TiC and VC in α–Fe [15].

	VC	TiC
Coherent strain	<15	<29
Interstitial site	-106	-58
C vacancy	116	125
Coherent interface	-6	48

first principle calculation, but calculation has not been performed for semi-coherent nor incoherent interface [15]. The calculated potential energies for hydrogen atoms trapped by TiC and VC are summarized in Table 1. TiC is expected to trap hydrogen in the coherent interface, whereas the C-vacancy in VC might be the trap site, but not be effective in the case of the high diffusion barrier. Computational material science is expected to be intensively exploited for the purpose of investigating the effective hydrogen trap sites.



a) b)

Fig. 9 a) Calculated interface energies of the coherent and semi-coherent NbC/ α-Fe interface as a function of the length of C_0, b) atomic configuration of the semi-coherent interface in the (110) plane [13]. The region of the dislocation core is positioned in the center of interface.

Future outlook

For the purpose of fully exploiting ICME, it is necessary to first brush up the fundamental research in the individual fields. Simultaneously, depending on the objectives, the relevant issues should be solved by linking and integrating the technologies in different fields. Furthermore, international collaboration will become more important in the future.

References

1. K.Ushioda, "Challenge for further strengthening of steels," Proc. 2nd Int. Symp. on Steel Science (ISSS-2009), Ed. by K. Higashida and N. Tsuji, ISIJ, Kyoto, (2009) , 39-48
2. K.Ushioda and H.Tsuchiya, "Fundamentals for controlling the microstructure and properties of cold rolled and continuously annealed sheet steels," *Trans. Ind. Ins. Met*, **6**6(2013), 655-664
3. K.Ushioda, S.Nakanishi, T.Morikawa, K.Higashida, Y.Suwa and K.Murakami, "Evolution of heterogeneous deformation structure and recrystallization texture of steel," *Mater. Sci. Forum*, **753**(2013), 58-65
4. S.Nakanishi, T.Morikawa, K.Higashida, H.Murakami, K.Kimura and K.Ushioda, "Effect of solute carbon content of microstructures of cold-rolled ferritic steel," *Tetsu-to-Hagane*, **98**(2012), 253-261
5. K.Kimura, K.Ushioda, J.Hamada, E.Ishimaru and A.Takahasi, "Recrystallization behavior of SUS 430 stainless steel containing hard second phase prior to cold-rolling," to be published.
6. J.Humphreys, P.Bate, A.Gholinia and I.Brough, "Measuring and modelling the microstructures of two-phase aluminium alloys after deformation," *Mater. Sci. Forum*,**715-716**(2012), 23-32
7. T.Takaki, A.Yamanaka, Y.Higo and Y.Tomita, "Development of phase-field model and

computational procedure during static primary recrystallization," *Jpn Soc. Mech. Engi. A*, **73**(2007), 482-489
8. A.Yamanaka, T.Takaki and Y. Tomita, "Simulation of austenite to ferrite transformation in deformed austenite by crystal plasticity finite element method and multi-phase-filed method," *ISIJ Int*., **52**(2012), 659-668
9. G.Shigesato, T.Fujishiro and T.Hara, "Boron segregation to austenite grain boundary in low alloy steel measured by aberration corrected SEM-EELS," *Mat. Sci. Engi. A*, **535**(2012), 358-365
10. H.Sawada, "First principles study of grain boundary embrittlement in Fe-Ni-S alloy," *Comp. Mater. Sci.*, **55**(2012), 17-22
11. S.Yoshida, K.Ushioda and J.Agren, "Kinetic model of the γ to α phase transformation at grain boundaries in Boron-bearing low-alloy steel," *ISIJ Int.*, **54**(2014), 685-692
12. J.Takahashi, K.Kawakami, Y.Kobayashi and T.Tarui, "The first direct observation of hydrogen trapping sites in TiC precipitation-hardening steel through atom prove tomography," *Scripta Mater.*, **63**(2010), 261-64
13. H.Sawada, S.Taniguchi, K.Kawakami and T.Ozaki, "First-principles study of interface structure and energy of Fe/NbC," *Modelling Simul. Mat. Sci. Eng*., **21**(2013), 045012
14. F-G Wei, T.Hara and K.Tsuzaki, "Nano-precipitates design with hydrogen trapping character in high strength steel," *ASM Int*., ISBN-13:978-1-61503-003-3, (2009), 448-455
15. K.Kawakami and T.Matsumiya, "Numerical analysis of hydrogen trap state by TiC and V_4C_3 in bcc-Fe," *ISIJ Int.*, **52**(2012), 1693-1697

3rd World Congress on Integrated Computational Materials Engineering (ICME 2015)
Edited by: Warren Poole, Steve Christensen, Surya R. Kalidindi, Alan Luo, Jonathan D. Madison, Dierk Raabe, and Xin Sun
TMS (The Minerals, Metals & Materials Society), 2015

ICME FOR PROCESS SCALE-UP: IMPORTANCE OF VERTICAL AND HORIZONTAL INTEGRATION OF MODELS

Gerald Tennyson, Rishabh Shukla, Saurabh Mangal, Savya Sachi, Amarendra K Singh

Tata Consultancy Services, Pune 411 013, India

Keywords: vertical-horizontal integration, process scale-up, multi-scale modelling, multi-phase modelling

Abstract

ICME will play a major role in reducing the lead time in development of a new product or component. One of the areas where ICME is likely to play a crucial role is process scale-up of mill products. Process scale-up of a mill product from laboratory to production stage is largely done through hit-and-trial and is a non-trivial exercise. It involves plant level trials which are expensive and time consuming. Use of ICME can significantly narrow down the design search space thereby reducing need for experimentation or plant trial, which in turn will lead to bringing down the cost and time of development. However many challenges need to be addressed to realize the full potential of ICME at an industrial scale. Manufacturing any product/ component involves a host of unit operations and the properties of the end product are intrinsically linked with final as well as intermediate processing steps. To link the material-processing-structure-performance matrix, there is a need to enhance models across various unit operations through multi-scale/multi-phase modelling and integration of models at various length scales. This allows for the information flow across various unit operations and thereby ensures horizontal integration of each process to simulate the entire manufacturing chain. This step is crucial in designing set points and quantifying the influence of various unit operations on end product performance. In this paper, we illustrate the vertical-horizontal integration of models through an example

Introduction

Modelling of materials processing and metallurgical operations has come a long way since its inception in the early seventies. Application of mathematical modelling in metallurgical process optimization, which began around the late seventies, has also progressed a long way. In current scenario, mathematical modelling and simulations are extensively used in several processing industries to either select a suitable design of equipment for their unit operations or to optimize the process operation. We illustrate the use of modelling and simulation technique for design and process optimization in steel industry with the help of few examples. In the recent past, steel industry has adopted major technological advances to compete with the challenges posed by new advanced materials. Steel manufacturers are striving to manufacture product mix with newer grade of steels (advanced high strength steel, for example) for improved properties. Manufacturing a steel product mix (rod, bar, sheet) involves a series of unit operations (see Figure 1), each having a significant influence on the final properties. Models to capture the effect of various phenomena occurring in a unit operation exist and are used frequently. We provide a gist of information on the current state of mathematical models for two of the unit operations, namely ladle refining and continuous casting.

Mathematical Models of Ladle Refining and Continuous Casting Operations

Ladle furnace receives steel form basic oxygen or electric arc furnace and is the key to maintain desired level of steel cleanliness and maintaining composition of alloying elements (Ni, Cr, Mn etc.) within a specified band. Steel cleanliness is assessed with respect to the amount and nature of

inclusions present and the level of tramp elements such as sulphur, oxygen and phosphorus in steel. The aim of refining operation is to facilitate deoxidation, superheat control, desulphurization, and inclusion removal to meet the specified requirements to meet the chemistry and cleanliness requirements at the end of ladle refining operation.. Mathematical models have been developed and employed to model the aforesaid phenomena. Singh et al. have developed a chemistry model to predict amount of additives to be added for maintaining desired steel and slag composition and a thermal model to account for the heat losses that occur during refining, thereby suggesting an arcing strategy to compensate for the same [1]. Population balance method (PBM) based inclusion evolution model to study the behaviour of inclusions and calculate final inclusion distribution coming out from ladle has been developed [2, 3]. To account for inclusions that are formed during course of refining, thermodynamic modelling is done and is coupled with PBM model. Lots of investigations are reported with respect to removal of sulphur during refining. Maintaining desired level of slag basicity and having favourable flow conditions to increase slag/steel interfacial area is of prime importance to facilitate sulphur removal. Models have been developed to study the effect of purging rate on sulphur removal [4]. Anderson et al. [5] talk about importance of slag compositional control for sulphur removal. They have developed model to calculate final sulphur content in steel with variation in the composition of ladle furnace slag. There are several other models addressing design related issues and other important aspects of ladle refining operation. We have provided a glimpse of some of the models that are used to understand various phenomena in ladle refining. We next describe few models used to understand few phenomena in continuous casting operation.

Caster receives steel from tundish and is a crucial step in formation of variety of steel products from liquid steel. The performance of casting operation is assessed in terms of productivity, quality parameters such as segregation, crack index, oscillation mark depth and cost of production. Different phenomena take place during casting that influences the aforesaid performance measures. Mathematical models have been developed to model these phenomena and design casting operation to meet the quality and productivity requirements. During casting, segregation of solutes takes place owing to difference in solubility limit in solid and liquid phase. Models are available to predict centre line segregation (CLS) in cast slab [6] and thereby designing the casting operation in a way to have severity of segregation within tolerable limit [7]. Thermo-mechanical models are available to predict surface and internal crack in a slab which occur as a result of thermal stresses developed during solidification. The model is used to optimize the cooling conditions in different segments of caster to produce a slab having cracks within acceptable limit. During continuous casting, inclusions get redistributed into columnar and equiaxed zone, which affect the quality of final product. Transition of morphology from columnar to equiaxed is thus of great importance for industry. Models are available to predict the location of columnar equiaxed transition and compute the relative proportions of columnar and equiaxed zone [8]. Another important phenomenon to occur during solidification is micro-segregation. Micro-segregation results in variation of solute concentration in the inter-dendritic region and lead to a situation favourable for formation of precipitates [9]. Models are available to capture micro-segregation during solidification, which is then used to predict evolution of precipitates during casting operation.

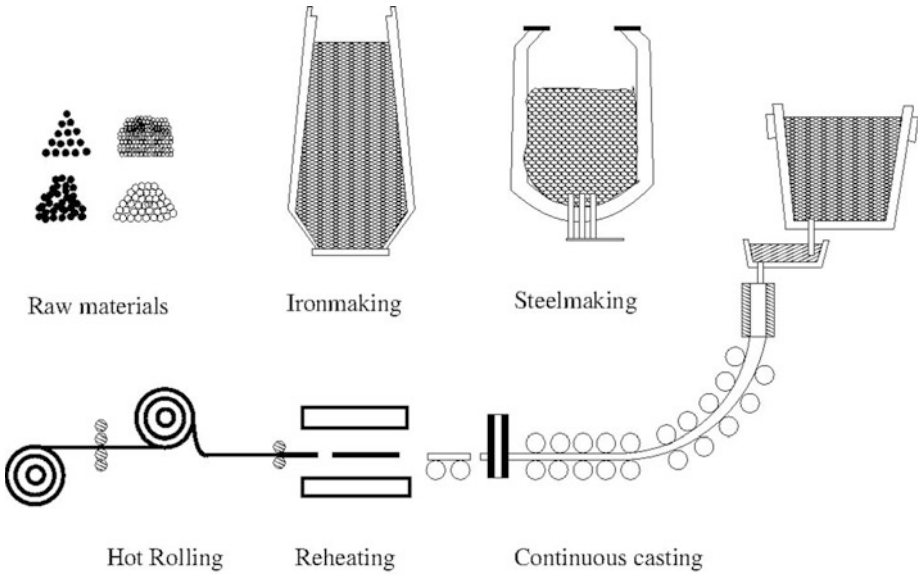


Figure 1. Schematic of operations in steel processing

The previous sections provide a glimpse of few mathematical models, used to study different phenomena occurring in two unit operations and address the associated challenges. The models that we have talked about previously are problem specific and are not studied in conjunction with the other phenomena. For example, desulfurization model is used to decide slag chemistry and argon purging during refining to optimize sulphur removal. However, while studying the same we do not consider deoxidation and inclusion evolution model. As a result, we may end up with desired sulphur content in steel but slippage may happen in other requirements (inclusion content, superheat etc.). This can be qualified by a study reported in [10], which says high purging rate is desired for sulphur removal which on other hand is detrimental for inclusion content as high purging lead to increase in oxygen pick up (increase in slag eye opening). Thus, a mathematical model used for process or design optimization of a unit operation should combine all important associated models to meet the conflicting requirements of productivity and quality of the product. It is important to note here that the product of ladle operation is steel melt for tundish and product of casting operation is slab or billet. Also, requirements of these products are well specified: Target chemistry and cleanliness in case of ladle refining and segregation level and other quality parameters in case of cast product. These have come about through trial and error and years of experience. In contrast, for process scale up of a new grade, the product requirements at the end of ladle refining, caster and other unit operations are not known apriori and need to evolve to meet the ***end product requirements.*** Thus, in ICME framework, modelling of unit operations is entirely different and the focus here is to generate information flow to immediate next and subsequent operations so as to relate these to end product requirements. For example, CLS model is used to design casting operation in a way so as to have severity of segregation within control (a requirement on slab). However, the CLS model does not give us any information on the composition profile in slab, which is very critical when we talk about deformation behaviour during rolling operation. In such a situation, a slab that has qualified after casting operation with respect to segregation level may not be suitable to be rolled. The silo-based study of unit operation is therefore not useful for development of steel product with specific properties.

Above discussions establish the need of ICME approach of model development and study. In ICME

approach, the flow of information from one unit operation to other is essential which enable us to carry out integrated study of each operation (termed horizontal integration) [11], unlike what is done in silo-based approach. The horizontal integration of unit operations requires information in far greater details, which will require modelling each phenomenon with a deeper insight. For example, requirement on steel product is put with respect to total oxygen content, which is a measure of inclusions present. Simple chemistry model is used to optimize ladle refining and predict operating conditions to meet total oxygen requirement. However, if we are doing an integrated study, further detailed models will be required to be able to provide information on chemical composition of inclusions, its type, morphology and size, as this information need to be passed on to the subsequent unit operation (during rolling). This will enable us to study the behaviour of inclusions of different size, shape and type during rolling. The integration of models for different phenomena and models at different length scales (termed as vertical integration) is required to establish the information required by subsequent unit operations. One such study in integrating computational thermodynamics with kinetics simulations on the strengthening mechanisms in magnesium alloys at elevated temperatures is done by Bryan et al.[12] The vertical integration is useful not only to obtain information required by subsequent operation but also help us to have a better understanding and process design of the corresponding unit operation as well. For example, integration of thermal, desulphurization and inclusion evolution model during refining helps us to explore the design set points of ladle operation to have a balance between these critical requirements. Focus in such a case is not to have maximum of one requirement but to achieve the specified target with respect to all three requirements. This is an aspect which remains untouched when doing optimization using an individual model.

Problem Statement

We have talked about importance of modelling and simulation in studying various processes. The essence of vertical-horizontal integration in ICME approach of development of materials, products and associated manufacturing processes is presented. Next, we explain the importance of proposed method of horizontal-vertical integration for solving a problem encountered during sheet manufacturing in steel industry. Suppose steel mill is involved in production of sheet with certain grade of steel. The operating constraints and process requirements are known to process designer as they are involved in sheet manufacturing day-in-day-out. However, if happens a scenario where owing to the changed performance and properties requirements, manufacturers are asked to produce sheet with a newer grade of steel with enhanced properties. This grade of steel is used to manufacture sheet at a laboratory scale, but now the challenge posed to sheet manufacturers is to scale-up the production from lab to an industrial scale. This requires exploring the design set points of each unit operation to produce the sheet with desired properties at a plant scale. One way of doing this is to resort to experimentation and plant trials, which is highly expensive and takes a lot of time (8-10 years for automotive materials). Other way is to use computational models for exploring the design set points, thereby reducing experimentation and time and cost incurred in the development. However, current models are problem specific and are developed to address issues of a particular phenomenon. The optimization of process using these models in isolation will not be a true representative of desired solution. The need of the hour is to use ICME approach of models integration to explore the solution space for production of a sheet. This requires exploring the design set points of involved unit operations, which in turn requires knowledge of operating constraints and requirements, which is not available for the case where sheet is being manufactured with a new grade of steel. The first task thus is to identify operating constraints and requirements for each unit operation, which is imposed by the subsequent unit operations as each process step is connected and information flows form one operation to the other. Schematic showing flow of information across the entire sheet manufacturing chain is presented in Figure 2. Identifying the aforesaid operating constraints process requirements requires having information about each spec in sufficient details. The vertical integration of models provide a way to obtain these information in

greater details (as is required), which is then passed across other unit operations to put constraints and requirements on them. This flow of information from one unit operation to other that allows for integrated study is termed as horizontal integration. For example, thermodynamic model for inclusion formation is integrated with PBM model and kinetics based model to calculate size, shape and type of inclusions. This information is passed on to subsequent operation and sets up a requirement for them. This way, we make use of vertical-horizontal integration to explore the design set points for manufacturing sheet with a new grade of steel. Next, we talk in greater detail about integration of models to obtain detailed information and making use of this information to predict the design set points of unit operation for manufacturing sheet with desired properties.

1. Integration of models to predict composition, size, shape and distribution of inclusions in the cast slab. This information is used in predicting the performance of final product (with respect to fatigue life) and studying the behaviour of slab during rolling.
2. Integration of models to predict micro-segregation and evolution of precipitates during solidification. This information is used to predict design set points of reheating operation.
3. Integration of models to obtain compositional profile across cast slab and precipitates. This information is used to predict design set points of reheating operation.

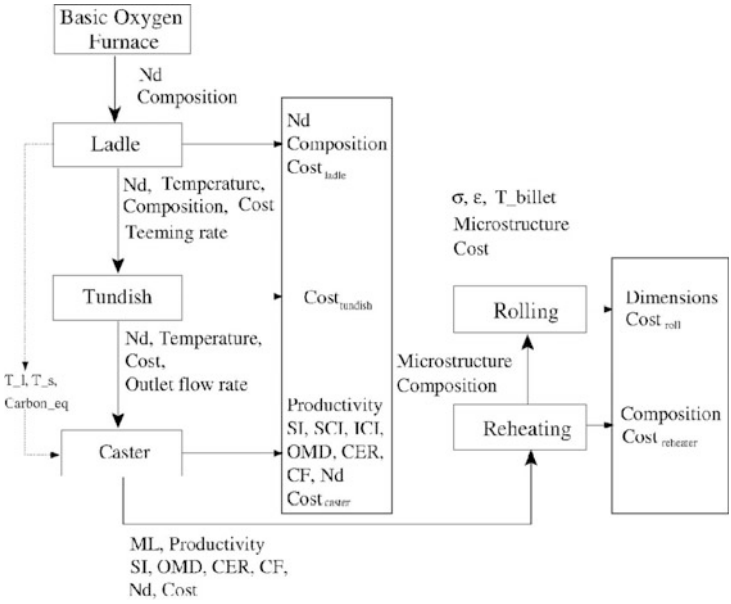


Figure 2. Flow of information across process chain

Illustrations of Vertical-Horizontal Integration

Models Integration for Inclusion Characterization

The aim of this vertical integration is to characterize inclusion distribution in the cast slab. The importance of this information and the modelling strategy adopted to obtain the same is elucidated. Let us consider a situation where the interest is to manufacture a sheet with specified fatigue life. Presence of inclusions significantly affects the fatigue life of sheet and inclusions in industry are measured in terms of total oxygen. The specification on fatigue life sets up a requirement to have

oxygen content in steel below 10 ppm. However, having total oxygen content below specified limit does not guarantee desired fatigue life as total oxygen is only a measure of amount of inclusions and do not tell anything about their composition, size, shape and distribution. Lot of study has been done to establish the effect of inclusions on fatigue life. Salajegheh et al. have carried out finite element simulation to study the effect of clustering of inclusions on performance of advance high strength steels during fatigue loading [13]. This establishes the importance of studying spatial distribution of inclusions in the cast slab. Performance of sheet during fatigue loading also depends on how the inclusions behave during rolling operation. The behaviour of inclusions during deformation depends on the type of inclusions, i.e., whether it is a hard inclusion or soft inclusion and how is it distributed in the matrix. Akash et al. [14] have studied the behaviour of hard and soft inclusions during hot rolling [14]. Luo in his thesis [15] has developed a model to study the behaviour of inclusions during rolling which in turn helps in carrying out rolling in a way so as to improve the properties of the final product. For example, he has reported a transition temperature for silicate inclusion below which these behave as non-plastic and plastic at temperature above. The studies reported above establish the importance of having inclusions information in far detail than merely using total oxygen as qualifying criteria. Next, we explain the modelling framework which can be utilized to obtain this information and preserve it to be utilized during rolling. Inclusions are largely removed or modified during ladle refining. Inclusions coming from basic oxygen furnace are removed and new inclusions, owing to refractory erosion and deoxidation, are formed during ladle refining. Information on size, shape, composition and distribution of inclusions has to be modelled during ladle refining. Integration of different models such as thermodynamic and kinetics model, population balance and fluid flow model (vertical integration), is used to obtain the aforesaid inclusion information. This information is then passed on to the next unit operation of continuous casting. Inclusions of different types and sizes from the ladle arrive at the caster with a given volume fraction and number density. Inclusions of all types are generally homogeneously distributed in the liquid steel but during solidification in caster, redistribution of inclusions occurs in the slab. It should also be noted that it is difficult to measure the distribution of inclusions in the cast slab even by a destructive examination of the slab. The difference between the solid and liquid densities causes the inclusions to either get trapped within the solid or transported to different sections in the cast. Inclusions in the melt are pushed towards the center mainly due to the moving columnar front. The spatial distribution of inclusion largely depends on the location of columnar-equiaxed transition (CET). However, not all the inclusions are pushed towards the CET. It has been established that the primary and secondary dendrite arm spacings (PDAS and SDAS) depend on the thermal gradient and the cooling rate respectively. In general, it is assumed that the inclusion whose size lies within the PDAS get engulfed by the growing columnar dendrites and those above, are pushed towards the center. By far, the most commonly used method to determine the location of inclusions is the model by Hunt [8], where it is possible to determine the location of the columnar to equiaxed transition zone using the thermal gradient and cooling rate information. We have developed a model based on Hunt's criteria on CET to predict inclusion size distribution in the cast slab. The number density of inclusions along with their sizes is shown in Figure 3. It is assumed at this point that the inclusions that are entering the cast (initial) get segregated in the center.

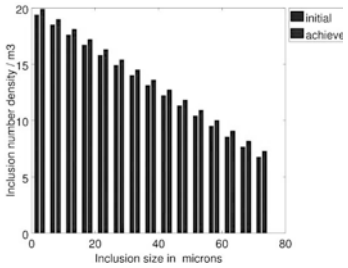


Figure 3. Variation in the inclusion number density as a function of its size

Further enhancements to the model are underway to determine the spatial variation of these inclusions throughout the cast section. We are incorporating the information on PDAS and SDAS into the current model (described above) to predict the spatial distribution of inclusions across the slab, which plays a significant role in determining the behaviour of slab during deformation and subsequently its properties.

We have obtained some information on inclusions which have been shown in the above figure. Following a similar vertical integration modelling strategy, we can obtain the detailed information on size, shape, composition, volume fraction and spatial distribution of inclusions. This information is then linked to models of rolling operation (horizontal integration) and is used to design the rolling process in a way so as to avoid any crack formation during deformation and to ensure attainment of desired fatigue life in the final sheet.

Models Integration to Predict Precipitates Evolution

The aim of this vertical integration is to obtain the information on level of micro-segregation and type, size and shape of precipitates formed during solidification. The importance of this information and the modelling strategy adopted to obtain the same is elucidated. Final properties of sheet depend on the microstructure and defects level present. Presence of certain precipitates in cast slab which is rolled, may have a tendency for crack formation and propagation and thereby increases the defect levels in the final sheet, more than the specified limit. It is essential to ensure such precipitates are not present in the slab to be rolled. This sets a target on reheating operation to ensure the precipitate requirements are met, so that no problems are encountered during rolling. We then need to obtain the information on size, shape and type of precipitates present in the slab that is reheated. The formation of precipitates during solidification depends on various factors such as localized variation in composition due to macro and micro-segregation, flow conditions, dendrite arm spacing etc. Lots of work has been done in past to understand micro-macro segregation, precipitation kinetics, fluid flow during solidification. However, these models have been used in isolation to optimize the casting operation with respect to a specific problem. This may help us to take care of a specific problem, but may lead to occurrence of others and we may not be able to capture the required information on size, shape and type of precipitates in sufficient detail. In this work, we illustrate vertical integration of different models (micro-macro segregation, precipitation kinetics, and fluid flow) to predict type, size and shape of precipitates formed (required by reheating operation as stated above).
Chemical composition of the alloy, cooling rate and thermal gradients decide the nature of precipitates that may form. Precipitation kinetics is modelled using a Scheil-Gulliver scheme, where solutal information is able to predict the type of precipitates that would form. Coupled with cooling rate, it is also possible to quantify the volume fraction of the precipitates that are evolving. Integrating precipitation kinetics and thermal model with a macro-segregation model is essential, because calculating precipitates evolution using nominal composition does not provide the exact representation of the actual scenario. During casting, as solidification proceeds, due to convective forces, macro-segregation causes the solutes to get redistributed along the length of the cast, thereby altering the nominal composition along the entire domain of the cast. The variation in the solute levels caused during macro-segregation further affects the solidification behaviour of the alloy. Different regions in the cast now tend to solidify differently. Solute rejection from the primary phase leads to micro-segregation. This also gets affected by the variation in the localized composition field caused by macro-segregation. We report evolution of precipitates MnS and NbC for both the aforesaid cases (with and without integration of macro-segregation model) to illustrate utility of vertical integration. In the absence of macro-segregation, solute segregation levels are uniform and we expect a uniform distribution of MnS and NbC depending on the cooling rate and segregation levels. The same is observed with the first model, which is evident from the horizontal lines for MnS and NbC (see Figure 4). However, when we use second modelling strategy (macro-