2001 TMS Fall Extraction and Process Metallurgy Meeting: Computational Modeling of Materials, Minerals, and Metals

What follows is the final technical program of the 2001 TMS Fall Extracting and Process Metallurgy Meeting: Computational Modeling of Materials, Minerals, and Metals which was scheduled for Setpember 23-26, 2001. Following the events of September 11, 2001, the ongoing difficulties associated with U.S. and international air travel, and the cancellation of nonessential travel by the employers of many attendees and presenters, this meeting has been postponed until further notice.

This technical program is being provided for archival purposes, and does not necessarily represent the planned symposia of the rescheduled conference.

At-A-Glance Technical Program

Monday AM

Monday AM Opening Plenary Session

Keynote
Multi-Physics Simulation of Metal Processing: Mark Samonds

Keynote
Computing the Dynamic Interaction of Magnetic Fields and Turbulent Conducting Fluids in Metals Processing: Koulis Pericleous

10:30 AM Break

Track A - CFD Modelling - I

10:45 AM
Simulation of Turbulent Flow and Particle Transport in the Continuous Casting of Steel: Q. Yuan; T. Shi; S. P. Vanka; B. G. Thomas

11:10 AM
CFD Modeling of the Hydrodynamics of Fluidization in the Sand Surrounding a Lost Foam Casting Pattern:Nathanael Harrison Hudson; Sushil Bhavnani; Ruel A. Overfelt

11:35 AM
Continuum Modelling of Granular Flows using PHYSICA, a 3-D Unstructured, Finite-Volume Modelling Framework: Nicholas Christakis; Mayur K. Patel; Mark Cross; John Baxter; Hadi Abou-Chakra; Ugur Tüzün

12:00 PM
Mathematical Model of Inclusion Removal during Steel Degassing: Michel Cournil; Frédéric Gruy; Pascal Gardin; Hubert Saint-Raymond

12:25 PM
Application of Coupled Continuum-Mesoscopic Computational Methods for the Simulation of Complex Fluids in Industrial Processes: Greg Glinski; Chris J. Bailey; Koulis Pericleous

Track B - Heat & Mass Transfer - I

10:45 AM
Heat Load Control of Blast Furnace Wall using Statistical Optimization Techniques: Tae-hwa Choi; Yong-hwan Chu; Chonghun Han

11:10 AM
Mathmatical Modeling and Experimental Verification of Assimilation of Exothermic Additions in Liquid Metals: Stavros A. Argyropoulos; Henry H. Hu

11:35 AM
A Model of the Cathode Dynamics in Electric Field-Enhanced Smelting and Refining of Steel: David Michael Dussault; Adam Powell

12:00 PM
A Mathematical Model for the Control of Metallurgical Properties of the Product Sinter: Ndabezinhle Manengi Dube; E. F. Vegman

12:25 PM
Modelling the Magnetostriction of Textured Ferromagnetic Materials with a Cubic Structure: Ruben Decocker; Leo Kestens; Yvan Houbaert

Monday PM

Monday PM Plenary Session

Keynote
Modelling and Process Optimization for Functionally Graded Materials: Dan Tortorelli

Track A - Optimization & Novel Methods

2:45 PM
Lattice Boltzmann Methods for Metallurgical Process Simulation: Christian Redl

3:10 PM
Viscosity Estimation Model for an Oscillating Cup Viscometer: Deming Wang; R. A. Overfelt

3:35 PM Break

3:50 PM
Numerical Optimization of Magnesium Reduction in a Modified Pidgeon Process: Alfred Yu; Henry Hu

4:15 PM
Deterministic and Regression Models of Nickel Oxide Reducing Roasting Process: V. M. Paretsky; A. V. Tarasov

4:40 PM
Integrating Computational Mechanics and Numerical Optimization for the Design of Material Properties in Electronic Packages: Stoyan Stoyanov; C. Bailey; M. Cross

5:05 PM
Computer-Aided Modeling and Control of Autogenous Copper Smelting Process: A. V. Tarasov; V. M. Paretsky

Track B - Melting & Solidification - I

2:45 PM
A Marker Chain Front Tracking Method for Modelling Meniscus Dynamics in the Al Ingot Casting Process: Fionn Iversen; Jon Arne Bakken; Stein Tore Johansen

3:10 PM
Computational Modeling of Heat Mass and Solute Transport in Directional Solidification Processes: Mohammed El Ganaoui; Patrick Bontoux

3:35 PM Break

3:50 PM
Computational Modelling of Freeze Layers in Smelting Processes: Andrew P. Campbell; Koulis A. Pericleous; Mark Cross

4:15 PM
Mathematical Modeling of Heat Transfer and Microporosity Formation in Die Cast A356 Wheels: P. Vo; D. Maijer; S. L. Cockcroft; M. A. Wells; C. Hermesmann

4:40 PM
Modelling Filters in Metal Casting Processes: Mark R. Jolly; Jean-Christophe Gebelin

5:05 PM
Computer Heat Transfer Model for Directionally Solidified Castings: Deming Wang; R. A. Overfelt

Tuesday AM

Tuesday AM Plenary Session

Keynote
Phase Field Methods for Modeling Microstructure: James A. Warren

Track A - Structure

9:45 AM
Microporosity Evolution and Interdendritic Fluid Flows during Solidification: Adrian S. Sabau; Srinath Viswanathan

10:10 AM
Cellular Automata Computer Model of Polycrystalline Plastic Deformation: Alexander V. Spuskanyuk; Yakiv E. Beygelzimer; Victor M. Varyukhin

10:35 AM Break

10:50 AM
Simulations of Microstructural Evolution: Martin E. Glicksman; Kegang Wang; P. Crawford

11:15 AM
Ab Initio Calculations of Theoretical Tensile Strength in Metals and Intermetallics: Mojmir Sob; Ligen Wang; Martin Friak; Vaclav Vitek

11:40 AM
Modeling of Interdendritic Strain and Interdendritic Cracking Phenomena during Dendritic Solidification Processes: Mostafa El-Bealy

Track B - Melting & Solidification - II

9:45 AM
Wax Injection in the Investment Casting Industry: Jean-Christophe Gebelin; Alexander Cendrowicz; Mark R. Jolly

10:10 AM
Micro/Macro Modeling of Ingot Cooling Processes for Ni-Cu-S Alloys: Apostle Mouchmov; Mark Cross; Koulis Pericleous

10:35 AM Break

10:50 AM
Comparison of Numerical Models of Solidification Behavior in Direct Chill Casting with Experiments: Christopher J. Vreeman; David Schloz; Matthew John M. Krane

11:15 AM
Two-Phase Predictive Finite-Element Flow Model for Semi-Solid Slurries: Frédéric Pineau

11:40 AM
CFD Simulation of Continuous Charging and Melting of Small Metallic Particles in a Melting Reactor: Stefan Pirker; Oszkar Biro; Philipp Gittler; Peter Mittag; Bernard Aigner

12:05 PM
Numerical Simulation of Wax Pattern Dimensions in Investment Casting: Adrian S. Sabau; Srinath Viswanathan

At-A-Glance Technical Program

Tuesday PM

Tuesday PM Plenary Session

Keynote
Computational Modelling of Metals Reduction Processes: Phil Schwarz

Track A - CFD Modelling - II

2:45 PM
Modelling of Raceway Hysteresis: Govind S. Gupta; S. Sarkar; M. G. Basavaraj; P. D. Patil

3:10 PM
Lifetime Prediction of Pneumatic Conveyor Bends with the Aid of Computational Models: Mayur K. Patel; Robert Hanson

3:35 PM Break

3:50 PM
A Parametric Study of Oxy-Fuel Burners in Secondary Aluminum Melting: Madhu Huggahalli; Neeraj Saxena; Ken Grieshaber; Jerry Bernardski; David Stoffel

4:15 PM
Computational Modelling of Vortex Formation in the Lead Refining Kettle: Suman Kumar; Chris Bailey; Mayur Patel; A. W. Piper; M. Cowling; R. A. Forsdick

4:40 PM
CFD Modeling of Solids Suspensions in Stirred Tanks: Lanre Oshinowo; André Bakker

5:05 PM
Water Model and Numerical Study on the Spout Height in a Gas Stirred Vessel: Diancai Guo; G. A. Irons

Track B - Thermo-Mechanical Modelling - I

2:45 PM
Thick Yield Surface: An Approach to the Processing of Computer Experiments on Polycrystalline Deformation: Yan E. Beygelzimer; Alexander V. Spuskanyuk; Victor Varyukhin

3:10 PM
Model for Stress, Temperature and Phase Transformation Behaviour of Steels on Run-Out Table in Hot Strip Mill: Heung Nam Han; Jae Kon Lee; Hong Jun Kim; Young-Sool Jin

3:35 PM Break

3:50 PM
Thermo-Mechanical Coupling Finite Element Analysis of Sheet Metal Extrusion Process: Zhanghua Chen; C. Y. Tang; T. C. Lee

4:15 PM
A Model for Calculating the Lankford Value in Sheet Steels: Sihai Jiao; C. Isaac Garcia; Anthony J. DeArdo

4:40 PM
Interfacial Modelling of Hot Rolling: A Probabilistic Approach: Sumitesh Das; Eric J. Palmiere; Ian C. Howard

5:05 PM
Computational Experiment in the Mechanics of Materials: Leon Mishnaevsky; Ulrich Weber; Nils Lippmann; Siegfried Schmauder

Wednesday AM

Wednesday AM Plenary Session

Keynote
Micro-Macro Modeling of Solidification Processes and Phenomena: Vaughan Voller

Track A - Heat & Mass Transfer - II

9:45 AM
A Steady State Electrothermic Simulation Analysis of a Carbothermic Reduction Reactor for the Production of Aluminium: Dimitrios I. Gerogiorgis; B. Erik Ydstie; Sridhar S. Seetharaman

10:10 AM
The Limitations of CFD Modelling for Furnace Atmosphere Troubleshooting: Paul F. Stratton; Neeraj Saxena; M. Huggahalli

10:35 AM Break

10:50 AM
Simulation of Internal Oxidation: Henrik Larsson; Martin Schwind; John Ågren

11:15 AM
Dynamic Model for a Vapor Recovery in Carbothermic Aluminum Process: Vianey Garcia-Osorio; Tor Lindstad; B. Erik Ydstie

11:40 AM
Computer Simulation of the Structure-Energetical Transformations at Combustion Synthesis in the Systems NiAl and TiAl: Mikhail D. Starostenkov; Gennadiy M. Poletayev; Alexandra S. Starostenkova

12:05 PM
Influence of Surface Pressure and Slag Layer on Bubble Bursting in Degasser Systems: Julie Cranga; Pascal Gardin; Didier Huin; Jacques Magnaudet

Track B - Melting & Solidification - III

9:45 AM
Computational Studies of the Control of Convection in Diamagnetic Liquids during Solidification with Magnetic Field Gradient: C. B. Seybert; J. W. Evans

10:10 AM
Methods for Approximating Discontinuous or Rapidly Changing Conductivity in Numerical Calculations: Vaughan Richard Voller

10:35 AM Break

10:50 AM
Modelling of the De-Waxing of Investment Cast Shells: Jean-Christophe Gebelin; Sam Jones; Mark R. Jolly

11:15 AM
The Swirling Effect in an Immersion Nozzle on the Flow in a Continuous Casting Mold: Shinichiro Yokoya; Sigeo Takagi; Manabu Iguchi; Katsukiyo Marukawa; Shigeta Hara

11:40 AM
Computational Modelling of Metals Extrusion and Forging Processes: A. J. Williams; T. N. Croft; M. Cross

12:05 PM
The Role of Orifice Shape in the Detection of Inclusions in Liquid Metals: Roderick I.L. Guthrie; Mei Li

Wednesday PM

Wednesday PM Plenary Session

Keynote
Computational Modeling of Thermo-Mechanical Phenomena: Christopher Bailey

Thermo-Mechanical Modelling II

2:45 PM
Mathematical Modeling of Mean Flow Stress during Hot Strip Rolling of Nb Microalloyed Steels: Ki Bong Kang; Sang Hyun Cho; John J. Jonas

3:10 PM
Modeling of Residual Stresses and Mechanical Behavior of Glass-Infiltrated Spinel Ceramic Composites: Anil Saigal; Edwin R. Fuller; Said Jahanmir

3:35 PM Break

3:50 PM
Simulation of Fatigue Stress Life (S-N) Diagrams for Ti-6Al-4V Alloy by Application of Artificial Neural Network: S. McShane; Savko Malinov; J. J. McKeown; Wei Sha

4:15 PM
Prediction of Lateral and Normal Force-Displacement Curves for Flip-Chip Solder Joints: Daniel Wheeler; Daniel Josell; James A. Warren; William E. Wallace

4:40 PM
Simulation of the Plastic Behavior during Mechanical Testing of Galvanized Steel using the Finite Element Method: Adriana Salas; Martha Patricia Guerrero Mata; Rafael Colás; René Garza

Technical Program Grid

	Monday-September 24		Tuesday-September 25		Wednesday-September 26	
	AM	PM	AM	PM	AM	PM
St. Tropez/Monte Carlo	Monday AM Opening Plenary Session	Monday PM Plenary Session	Tuesday AM Plenary Session	Tuesday PM Plenary Session	Wednesday AM Plenary Session	Wednesday PM Plenary Session
St. Tropez	Track A - CFD Modelling - I	Track A - Optimization & Novel Methods	Track A - Structure	Track A - CFD Modelling -II	Track A - Heat & Mass Transfer - II	Thermo-Mechanical Modelling - II
Portofino/Marseilles	Track B - Heat & Mass Transfer - I	Track B - Melting & Solidification - I	Track B - Melting & Solidification - II	Track B - Thermo-Mechanical Modelling - I	Track B - Melting & Solidification - III	

2001 FALL EXTRACTION AND PROCESS METALLURGY MEETING: COMPUTATIONAL MODELING OF MATERIALS, MINERALS & METALS PROCESSING SYMPOSIUM
September 23–26, 2001
San Diego, California

Monday AM
Opening Plenary Session
9:00 AM–10:30 AM

Monday AM — Room: St. Tropez/Monte Carlo
September 24, 2001 — Location: Hilton San Diego Resort

Session Chairs: Mark Cross, The University of Greenwich, Centre for Numerical Modelling & Process Analysis, Old Royal Naval College, 30 Park Row, Greenwich, London SE10 9LS UK; James W. Evans, University of California, Dept. of Matls. Sci. & Min. Eng., 585 Evans Hall, Berkeley, CA 94720-1760 USA

Keynote
Multi-Physics Simulation of Metal Processing: Mark Samonds[1]; [1]UES Software, Inc., 175 Admiral Cochran Dr., Annapolis, MD 21401 USA

Manufacturing processes which involve liquid to solid and solid state transformations in metals encompass a wide variety of physical phenomena. The past twenty years have seen a steady evolution in the complexity and scope of numerical models of these processes, beginning with thermal analyses without phase change. Recently, a few software packages have become available which have true multi-physics capabilities. This permits the treatment of thermal, fluids, stress, electromagnetic, chemical reaction and microstructure development aspects altogether in a fully coupled simulation. This paper will consider various aspects of these types of models.

Keynote
Computing the Dynamic Interaction of Magnetic Fields and Turbulent Conducting Fluids in Metals Processing: Koulis Pericleous[1]; [1]University of Greenwich, Greenwich Maritime Campus, Queen Mary Ct., Rm. 361, Greenwich, London SE10 9LS UK

Magnetic fields have many actual applications in the metals processing industry. Externally applied magnetic fields give rise to electromagnetic (Lorentz) forces formed by the cross product JxB, between the induced current density J and the magnetic field density B. When the metal is in liquid form, the Lorentz force generates motion in the fluid which in applications of practical interest becomes turbulent. In modelling terms, the Lorentz force appears as a source in the momentum equations. In addition, the induced current generates heat (Joule heating) in the metal that is in proportion to J^2, with a corresponding sou rce of heat in the energy equation. Whether as heat or as a force, these effects represent action at a distance–a most useful attribute when dealing with hot metal. The Lorentz force is used to stir solidifying alloys, pump liquid metal in conduits, dampen the flow in the meniscus of a continuous caster, levitate metal drops, induce artificial gravity conditions in suspensions or contain liquid metal. Elsewhere, the Lorentz force may be a by-product of some other operation, so leading to wave excitation in aluminium electrolysis cells, or altering the shape of the weld pool in arc welding. Joule heating is most commonly used with applied AC fields, to melt metal in induction furnaces. The author and his colleagues have been involved in the modelling of most of these processes in the past decade. Modelling is not however straightforward, since most of the examples mentioned represent genuine *multi-physics* challenges. There is a strong coupling between the flow field and electromagnetic field. The addition of a dynamically varying metal free surface and the moving solidus front means the flow, heat and electromagnetic fields need to be computed simultaneously. In situations involving metal containment, the metal free surface position is governed by the interplay of gravity, Lorentz force, surface tension and fluid inertia. Since all the interesting effects often happen in thin boundary layers at the surface due to the *skin effect*, mesh generation and mesh control during the computation become non trivial problems that need to be addressed. This paper presents a review of numerical methods used to model droplet levitation, semi-levitation melting and cold crucible induction melting of metals. The first method is based on spectral collocation techniques and the second is the traditional FV approach. Steps taken to validate the computations and typical transient results are also given.

10:30 AM Break

Track A - CFD Modelling - I

Monday AM
September 24, 2001

Room: St. Tropez
Location: Hilton San Diego Resort

Session Chairs: Mark Samonds, UES Software, Inc., 175 Admiral Cochran Dr., Annapolis, MD 21401 USA; Mayur Patel, University of Greenwich, Ctr. of Numcl. Modlg. & Proc. Analy., London SE10 9LS UK

10:45 AM

Simulation of Turbulent Flow and Particle Transport in the Continuous Casting of Steel: Q. Yuan[1]; T. Shi[1]; S. P. Vanka[1]; B. G. Thomas[1]; [1]University of Illinois at Urbana–Champaign, Dept. of Mechl. & Indl. Eng., 1206 W. Green St., Urbana, IL 61801 USA

The quality of continuous cast steel is greatly affected by fluid flow in the mold region, especially involving transient phenomena. Mathematical models are being applied to investigate many different aspects of these phenomena, but their accuracy must be validated before they can be applied with confidence. As part of a long-term effort to develop and apply comprehensive models of the continuous casting process, this work evaluates the relative accuracy of models of three different fluid flow phenomena in continuous casting through comparison with measurements. Firstly, transient flow simulations of velocities in the mold region are compared with digital particle image velocimetry (PIV) measurements in a single phase water model. Large-eddy simulations (LES) are found to reasonably match the flow measurements, including transient flow variations, except at long time scales, which could not be modeled owing to the excessive computation costs. The standard K-e model produced very good agreement with time-averaged velocities for relatively little computation time, although it is inaccurate at predicting the transient variations. Secondly, particle trajectory calculations are compared with water model measurements to study the distribution and flotation removal of inclusion particles. The LES model was able to match the measurements both qualitatively and quantitatively. Thirdly, steady, multiphase flow computations are compared with flow patterns observed in both a water model and an operating steel caster with argon gas injection. For the same conditions, the water model and steel caster produced very different flow behavior. The computational model was able to match the measured flow patterns in both cases. This work suggests that computational flow modeling has the potential to match real processes as well or better than water models, especially when complex related phenomena such as particle motion and multiphase flow are involved. Much work is still needed to further improve the models and to apply them in parametric studies.

11:10 AM

CFD Modeling of the Hydrodynamics of Fluidization in the Sand Surrounding a Lost Foam Casting Pattern: Nathanael Harrison Hudson[1]; Sushil Bhavnani[1]; Ruel A. Overfelt[1]; [1]Auburn University, Dept. of Mechl. Eng., 213 Ross Hall, Auburn University, AL 36849 USA

In the aerospace and automotive industries, shapes arise which require casting. The problem with these cast parts is the empiricism and expense in developing an efficient casting process. There has been an interest in using the fluidized bed to allow sand to better encapsulate the complicated surface geometry of a lost foam pre-casting mold. Fluidization helps to eliminate the voids in the sand and improves the integrity of the casting. At issue is the hydrodynamics of the sand and air around the pre-casting mold. The software PHOENICS, employing a two-fluid approach, is used to simulate the flow of sand and air as interpenetrating continua. The kinetic theory of granular flow for the sand phase is incorporated into the re-compilable PHOENICS code. The results of this study consist of voidage patterns and the velocity components of the respective phases around the pre-casting submerged in a two-dimensional fluidized bed. The model is benchmarked against experimental voidage patterns without a foam pre-casting and to some trials with a pre-casting. The final test consists of a series of computer runs with an obstacle submerged in the bed at various aspect ratios of length to width.

11:35 AM

Continuum Modelling of Granular Flows using PHYSICA, a 3-D Unstructured, Finite-Volume Modelling Framework: Nicholas Christakis[1]; Mayur K. Patel[1]; Mark Cross[1]; John Baxter[2]; Hadi Abou-Chakra[2]; Ugur Tüzün[2]; [1]University of Greenwich, Ctr. of Numcl. Modlg. & Proc. Analy., Sch. of Compg. & Mathl. Scis., 30 Park Row, London SE10 9LS UK; [2]University of Surrey, Dept. of Cheml. & Proc. Eng., Guildford, GU2 5XH Surrey, UK

In recent years significant effort has been put in using Continuum Mechanics for the description of granular flows. Although these models are partially successful in capturing some flow characteristics, they lack essential information on material properties, which are needed to account for the interactions between different particles. Thus, they are incomplete and can not be used to describe processes such as hopper filling/emptying and pneumatic conveying, where particle-particle interactions can lead to phenomena such as segregation, degradation and agglomeration. In this paper, a 3-D unstructured Finite-Volume framework is presented, which employs interface tracking techniques (VOF/SEA algorithms) to determine the material-air interface. Separate routines are employed to perform the tracking of the individual material components of the granular mixture in the bulk. Various transport processes, arising from the micro-mechanical properties of the different particle species in the granular mixture, can be obtained through kinetic theory. The transport coefficient(s) of each of the individual species can be determined and analysed in a micro-mechanical framework and the transport process parametrised in the form of constitutive model. These models provide the continuum theory with information on the micro-mechanics. This work describes in detail the numerical schemes employed in the Continuum Mechanics framework and the micro-mechanical

parametrisations that are implemented in the transport equations. Model predictions for different flow conditions and comparisons with experimental data are presented and conclusions are drawn on the model capability to realistically predict and quantify the main characteristics of granular flows.

12:00 PM

Mathematical Model of Inclusion Removal during Steel Degassing: Michel Cournil[1]; Frédéric Gruy[1]; Pascal Gardin[2]; Hubert Saint-Raymond[3]; [1]Ecole des Mines de Saint-Etienne, SPIN Div., 158 Cours Fauriel, Saint-Etienne, Cedex 2 42023 France; [2]IRSID, Themef, Voie Romaine, BP 30320, Maizières-lès-Metz, Cedex 57283 France; [3]IRSID, PCMO, Voie Romaine, BP 30320, Maizières-lès-Metz, Cedex 57283 France

The control of inclusion elimination is getting more and more important to obtain clean steel. But having a predictive tool is still a challenge, because the number of phases is important in steelmaking industry: liquid steel, slag layer, bubbles and inclusions (with a large range of composition and rheology). The paper presents the methodology which is developed at IRSID to predict oxygen content evolution during RH degassing. The main mechanisms which have to be considered are: -inclusion growth by turbulent aggregation of elementary inclusions (keeping in mind that liquid steel is a non-wetting medium for inclusions); the difficulty is to express collision efficiency for alumina particles, -inclusion removal by flotation; the difficulty for alumina clusters stems from the complex morphology of particle; fortunately, the use of fractal concept makes it possible to cope with this problem. The proposed paper describes the general modelling of inclusion removal taking into account the previous mechanisms. Hydrodynamic parameters are obtained by means of Fluent CFD package and a specific coding is developed for cluster growth. Influence of different parameters (fractal dimension, argon flow rate) on time-dependant inclusion size distribution is given.

12:25 PM

Application of Coupled Continuum-Mesoscopic Computational Methods for the Simulation of Complex Fluids in Industrial Processes: Greg Glinski[1]; Chris J. Bailey[1]; Koulis Pericleous[1]; [1]University of Greenwich, 30 Park Row, Greenwich SE10 9LS UK

Recent advances in new computational modelling techniques such as Lattice-Boltzmann and Dissipative Particle methods offer the prospect of simulating complex fluids such as colloidal and dense suspensions in industrial processes. These methods provide a means to overcome challenges that arise in modelling such fluids due to the disparate temporal scales present. These methods are termed mesoscopic methods as they lie between computational intense molecular dynamics and traditional macroscopic CFD methods. This paper will discuss the use of the methods to simulate the movement and subsequent processing of solder paste material in electronic component manufacture. Results will be presented that show how these methods are coupled within a macroscopic CFD code to provide detailed predictions of solder paste deposition onto a printed circuit board. Comparisons between the model results and experimental data will also be presented.

Track B - Heat & Mass Transfer - I

Monday AM
September 24, 2001

Room: Portofino/Marseilles
Location: Hilton San Diego Resort

Session Chairs: Koulis Pericleous, University of Greenwich, Greenwich Maritime Campus, Greenwich, London SE10 9LS UK; Stavros A. Argyropoulos, University of Toronto, Dept. of Metall. & Matls. Sci., 184 College St., Toronto, Ontario M5S 3E4 Canada

10:45 AM

Heat Load Control of Blast Furnace Wall using Statistical Optimization Techniques: Tae-hwa Choi[1]; Yong-hwan Chu[2]; Chonghun Han[2]; [1]Pohang Iron and Steel Company(POSCO), Techl. Rsrch. Labs./Iron & Steel Making Rsrch. Grp., 1 Goedong-dong, Nam-gu, Pohang-shi, Gyungbuk 790-785 Korea; [2]Pohang University of Science and Technology, Dept. of Chem. Eng., 31 san Houja-dong, Nam-gu, Pohang-shi, Gyungbuk 790-300 Korea

In the blast furnace, various complex phenomena take place including mass transfers, heat transfers, a lot of reactions and phase equilibriums, but systems of these phenomena are not found out clearly even until now. Consequently, it is very difficult to make fundamental models on these systems, which results in the operation based on the heuristics of industrial operators by changing operating condition little by little due to ignorance of the optimum point. However, since this method is not systematic, we propose statistical optimization technique based on analysis of historical data and empirical model building. In this approach, we first find the variables which must be optimized and the manipulated variables to adjust those response variables. Next, we collect the necessary data for these variables after preprocessing such as removal of noise and outlier. Finally, we construct empirical models describing the patterns of response variables in terms of manipulated variables by PLS regression method, and then these models are used as objective functions for entire optimization problem. By using appropriate optimization algorithm, this multi-objective optimization problem is solved, which gives us the compromising optimum operating condition considering all response variables from the past operating conditions.

11:10 AM

Mathmatical Modeling and Experimental Verification of Assimilation of Exothermic Additions in Liquid Metals: Stavros A. Argyropoulos[1]; Henry H. Hu[2]; [1]University of Toronto, Dept. of Metall. & Matls. Sci., 184 College St., Toronto, Ontario M5S 3E4 Canada; [2]University of Windsor, Dept. of Mech., Automot. & Matls. Eng., 401 Sunset Ave., Windsor, Ontario N9B 3P4 Canada

The assimilation of exothermic additions in liquid metals exhibit an array of unique coupled heat, mass and momentum transport phenomena. The phenomena are further complicated with the presence of a moving boundary. In this paper a mathematical model will be described which solves these coupled complex phenomena. The SIMPLER algorithm was employed to solve numerically the perti-

nent partial differential equations. The computational results indicated that the exothermic heat of mixing leads to a rapid increase of temperature around the moving boundary, which produced an enhanced convective flow in the liquid phase. The intensification of fluid flow around the moving boundary resulted in an acceleration of the melting process. An extensive verification of the mathematical model was carried out and will be described in the paper. First, in a low temperature physical model consisting of ice immersion in different sulfuric acid solutions. In this physical model, both temperature and velocity measurements were carried out. The model results were compared with experimental measurements and they were found to be in good agreement. Second, in a high temperature work involving assimilation of silicon in high carbon liquid iron. The model was also applied to predict fluid flow, heat and mass transfer for this high temperature experiments and a reasonable agreement was obtained. In addition new dimensionless heat transfer correlations that quantify these complex phenomena will be presented.

11:35 AM
A Model of the Cathode Dynamics in Electric Field-Enhanced Smelting and Refining of Steel: David Michael Dussault[1]; Adam Powell[1]; [1]Massachusetts Institute of Technology, Matls. Sci. & Eng., 77 Massachusetts Ave., Rm. 4-117, Cambridge, MA 02139 USA

A mathematical model of coupled diffusion, electrochemical reactions and fluid dynamics at the cathode in electric field-enhanced smelting and refining of steel is developed using the Navier-Stokes equations and the phase field method. Experimental evidence indicates that the reaction rate is limited by ferrous ion transport to the cathode, resulting in a Mullins-Sekerka instability at the slag-metal interface and the growth of liquid iron fingers into the liquid slag. The differential equations are discretized using finite differencing with a uniform mesh, and the resulting system of nonlinear equations is solved using a multidimensional Newton-Krylov method. Presented are the formulation and two dimensional results, and issues expected to arise on extension to three dimensions are discussed.

12:00 PM
A Mathematical Model for the Control of Metallurgical Properties of the Product Sinter: Ndabezinhle Manengi Dube[1]; E. F. Vegman[2]; [1]University of Zimbabwe, Fac. of Eng., Dept. of Metall. Eng., PO Box MP167, Mount Pleasant, Harare, Zimbabwe; [2]Institute of Steel and Alloys, Moscow, Russia

In the conventional practice of sintering, the quality of the product sinter down the cross-section of the bed is quite variable,with the top layer consisting of weak sinter and the bottom layer, strong over-fused sinter of poor reducibility. This points to a variable distribution of the heat balance in the sintering process down the sinter bed. This causes losses in the productivity of the sinter machine and the blast furnace. The experienced phenomenon caused by varying input of regenerated heat requires a zonal approach to the study of the sintering process with the aim of producing a uniform quality of the sinter cake. The current work includes a mathematical model that would make possible optimization of multiple-layer sintering and segregation technologies. It is based on a zonal heat balance. This calculation method presents the following prospects: 1. The minimum theoretically possible coke fines consumption during the sintering of any type of iron ore fines can be established. The optimum difference between the coke fines rates in the top and bottom layers during multiple-layer sintering should be easily determined with the aid of this model. 2. On the basis of this model an automatic control system for the coke rates in the top and bottom layers during two-layer sintering is possible. 3. The model can be used to control the quality (chemical, physical and metallurgical) of the sinter in any point down the sinter bed since the data input includes basicity, combustion zone temperature, and FeO content in the product sinter.

12:25 PM
Modelling the Magnetostriction of Textured Ferromagnetic Materials with a Cubic Structure: Ruben Decocker[1]; Leo Kestens[1]; Yvan Houbaert[1]; [1]University Ghent, Metall. & Matl. Sci., Technologie-park 9, Ghent, East-Flanders 9052 Belgium

A magneto-elastic model is presented to calculate the orientation dependence of the magnetostrictive strain, observed at saturated magnetization in ferromagnetic materials with a cubic crystal structure and an arbitrary crystallographic texture. The formula of Becker and Döring is used to express the anisotropy of magnetostriction for a single crystal. In order to simulate the macroscopic average magnetostriction of a polycrystalline aggregate (with an arbitrary texture) the Reuss assumption of the elasticity theory was applied. According to this assumption the various orientations of the polycrystal can deform without constraints, producing local strain incompatibilities in the microstructure but observing a total stress equilibrium. The macroscopic strain is calculated as the weighted average of the individual strains of all orientations composing the polycrystal. The weight factors are determined by the volume fractions of the corresponding orientations of the given texture, which can be measured by standard X-ray diffraction techniques. The model is applied to simulate the variation of magnetostriction (at saturation) with respect to the rolling direction for a standard grade of non-oriented electrical steel. A brief comparison with experimental data allows validating the basic model assumptions.

Monday PM Plenary Session
2:00 PM–2:45 PM

Monday PM
September 24, 2001

Room: St. Tropez/Monte Carlo
Location: Hilton San Diego Resort

Session Chair: Vaughan Voller, University of Minnesota, Saint Anthony Falls Lab., Minneapolis, MN 55414-2196 USA

Keynote
Modelling and Process Optimization for Functionally Graded Materials: Dan Tortorelli[1]; [1]University of Illinois–Urbana, Dept. of Mechl. & Indl. Eng., 350 MEB, MC 244, 1206 W. Green, Urbana, IL 61801 USA

We optimize continuous quench process parameters to produce functionally graded aluminum alloy extrudates.

To perform this task, an optimization problem is defined and solved using a standard nonlinear programming algorithm. Ingredients of this algorithm include 1) the process parameters to be optimized, 2) a cost function: the weighted average of the precipitate number density distribution, 3) constraint functions to limit the temperature gradient (and hence distortion and residual stress) and exit temperature, and 4) their sensitivities with respect to the process parameters. The cost and constraint functions are dependent on the temperature and precipitate size which are obtained by balancing energy to determine the temperature distribution and by using a reaction-rate theory to determine the precipitate particle sizes and their distributions. Both the temperature and the precipitate models are solved via the discontinuous Galerkin finite element method. The energy balance incorporates nonlinear boundary conditions and material properties. The temperature field is then used in the reaction rate model which has as many as 105^{o} of-freedom per finite element node. After computing the temperature and precipitate size distributions we must compute their sensitivities. This seemingly intractable computational task is resolved thanks to the discontinuous Galerkin finite element formulation and the direct differentiation sensitivity method. A three-dimension example is provided to demonstrate the algorithm.

Track A - Optimization & Novel Methods

Monday PM
September 24, 2001

Room: St. Tropez
Location: Hilton San Diego Resort

Session Chair: Dan Tortorelli, University of Illinois–Urbana, Dept. of Mechl. & Indl. Eng., Urbana, IL 61801 USA

2:45 PM
Lattice Boltzmann Methods for Metallurgical Process Simulation: Christian Redl[1]; [1]Mining University Leoben, CD-Lab. Appl. Comptnl. Thermofluid-dyn., Franz-Josef-Strasse 18, Leoben 8700 Austria

The Lattice Boltzmann Method (LBM) solves fluid dynamics problems based on a discrete mesoscopic approach. It is based on the Lattice Boltzmann equation which is a special discretisation of the continuous Boltzmann equation. Its principle advantage is that it can handle complex physical phenomena (like interaction between different components and surface effects), complicated boundary and initial conditions very well, free from many gridding and stability constraints that plague conventional numerical methods used for fluid flow simulations. The LBM algorithm has a simple structure and acts locally, which is favourable for parallel computing. Complex structures like porous media can be resolved directly. Its potential for metallurgical process simulations is demonstrated in the present study which is concerned with the simulation of the flow in a copper winning electrolysis cell. The electrolyte is modelled as the carrier fluid and the oxygen is considered via a so called active scalar equation. The modelling of buoancy, momentum exchange and the free surface requires special effort. The results of the simulation are validated against experimental data obtained by Laser-Doppler-Anemometry. Despite the simplifications made, good agreement was found.

3:10 PM
Viscosity Estimation Model for an Oscillating Cup Viscometer: Deming Wang[1]; R. A. Overfelt[1]; [1]Auburn University, Dept. of Mechl. Eng., 201 Ross Hall, Auburn University, AL 36849 USA

Viscosity measurements of molten alloys become more and more important in modern metallurgy engineering. Lack of the viscosity data of many new alloys hampers many CAD computer codes to apply in casting manufactures. The oscillating cup viscometer has become a dominant technique to measure the viscosities of high temperature molten metals. Unfortunately, the viscosity estimation model from the observed logarithmic decrement and period of the oscillation is very complicated. There are still large discrepancies of viscosity estimation values between using different measurement facilities or using different viscosity estimation models for a same molten metal. The purpose of the paper is to evaluate the accuracy of an oscillating cup viscometer in Auburn University. Two well known viscosity estimation models, Roscoe's and Torklep's equations, are discussed and compared viscosity for different alloys. The theoretical literature for the fluid flow inside an oscillating cup is reviewed and a more accurate working equation for Auburn oscillating cup viscometer is developed. Some design parameters of the oscillating cup viscometer which also directly affect the accuracy of viscosity estimation by using the working equation are discussed. In addition, applications and experimental measuring data are presented in the paper for several different commercial alloys, such as aluminum alloys: A319, A356 and A201, nickel-base super alloys: In713 and In718, and casting irons, C40 Gray Iron and Ductile Iron.

3:35 PM Break

3:50 PM
Numerical Optimization of Magnesium Reduction in a Modified Pidgeon Process: Alfred Yu[1]; Henry Hu[2]; [1]Nanjing Welbow North America Office, 601-969 Felix Ave., Windsor, Ontario N9C 4C7 Canada; [2]University of Windsor, Mechl. & Matl., 401 Sunset, Windsor, Ontario N9B 3P4 Canada

A numerical model of heat and mass transfer in the retort was set up to simulate and optimize the reduction phenomena in the process of Pidgeon magnesium reduction. The simulations were run to determine the effect of varying processing parameters on the magnesium reduction time. The model predicted the temperature distributions, the heating curves, the recovery ratio of magnesium, and the total process time. The predictions were used to optimize the magnesium reduction process, the dimensions of retort, the shapes of materials, and reaction cycle. Demo operation shows that, with application of the optimizations, significantly production capacity increases in the same furnace, reduction period decreases, energy consumption decreases.

4:15 PM
Deterministic and Regression Models of Nickel Oxide Reducing Roasting Process: V. M. Paretsky[1]; A. V. Tarasov[1]; [1]State Research Center of Russian Federation, State Rsrch. Inst. of Non-ferrous Metals "Gintsvetmet", 13, Acad. Korolyov St., 129515 Moscow, Russia

A mathematical model of the low-temperature (soft) nickel oxide reduction (SNOR) in a tubular kiln has been developed including an equation describing changes in the nickel oxide content of the solid material along the length of the kiln; an equation describing the changes in the content of reagents ensuring nickel reduction (i.e., hydrogen and carbon monoxide) in the gas phase along the kiln length; as well as the temperature along the kiln length. The kinetic relationships used for the development of the model had been determined based on experiments conducted specially for this purpose. Model investigations were conducted to determine the distribution of such parameters along the length of the kiln as the contents of metals oxides in the solids, partial pressure of hydrogen and carbon monoxide, variations of the temperature depending on the SNOR process conditions, including the kiln rotation speed. Based on the data obtained, a simplified regression model of the reducing roasting process was developed.

4:40 PM
Integrating Computational Mechanics and Numerical Optimization for the Design of Material Properties in Electronic Packages: Stoyan Stoyanov[1]; C. Bailey[1]; M. Cross[1]; [1]University of Greenwich, Sch. of Compg. & Mathl. Sci., 30 Park Row, Greenwich, London SE10 9LS UK

Silicon components containing transistor circuitry are at the heart of electronic products such as computers, mobile phones, etc. These components are connected to printed circuit boards (PCB's) using solder material that acts as the conductor for both electricity and heat. During the lifetime of a product it will undergo many thermal cycles where the chip becomes hot during product operation and then cools when the product is switched off. At the product design stage engineers undertake thermo-mechanical simulations to predict the thermal stress in the solder joints due to this thermal cycle and to ensure that the stress magnitude will not result in early fatigue-type failure. The design engineer's aim is to identify component parameters which ensure that the solder will survive beyond a certain number of thermal cycles. The aim of integrating computational mechanics and optimization tools together is to speed up dramatically the design process. From viewpoint of a design engineer in the electronics manufacturing sector, these tools can be used to quickly estimate key design parameters (i.e. material properties, product dimensions, etc.) that will guarantee the required product performance. In this paper a modeling approach coupling computational mechanics techniques with numerical optimization is presented and demonstrated. The integrated modeling framework is obtained by coupling the multi-physics framework–PHYSICA–with the design optimisation tool–VisualDOC. Thermo-mechanical simulations are presented that predict the creep strains in solder material. Different numerical optimization procedures: Direct and Response Surface based optimization plus Design of Experiments, are tested as a part of this modeling framework.

5:05 PM
Computer-Aided Modeling and Control of Autogenous Copper Smelting Process: A. V. Tarasov[1]; V. M. Paretsky[1]; [1]State Research Center of Russian Federation, State Rsrch. Inst. of Non-ferrous Metals "Gintsvetmet", 13, Acad. Korolyov St., 129515 Moscow, Russia

Based on theoretical and experimental studies into the specific features of the mechanism, kinetics, aerodynamics and heat transfer parameters of the flame-type oxidation of metal sulfides in a stream of technical-grade oxygen, a three-dimensional deterministic mathematical model of an oxygen-flame smelting furnace has been developed on the basis of the zonal method for computation of heat exchange. The model is presented in the form of equations taking into consideration the radiation component of the selective radiation, the convection component of mass transfer between the space and surface zones, heating of charge particles due to heat conductivity, accretions formation on a multilayer refractory lining with inserted cooling elements. The adaptation of the model for a full-scale furnace has demonstrated the possibility for its use for computation of main smelting process parameters. Multifactor model investigations were conducted and the results obtained were applied using statistical methods for development of a simplified computational regression model describing the interrelation of the main output parameters: temperatures of flame, lining, slag and off-gas; heat fluxes to the lining; thickness of accretions; heat removed by cooling elements; copper content of matte. On the basis of this model, a block diagram of the algorithm was developed for control of the thermal conditions of the furnace, as well as the control algorithm itself.

Track B - Melting & Solidification - I

Monday PM — Room: Portofino/Marseilles
September 24, 2001 — Location: Hilton San Diego Resort

Session Chairs: Vaughan Voller, University of Minnesota, Saint Anthony Falls Lab., Minneapolis, MN 55414-2196 USA; Matt Krane, Purdue University, Dept. of Matls. Eng., West Lafayette, IN 47907 USA

2:45 PM
A Marker Chain Front Tracking Method for Modelling Meniscus Dynamics in the Al Ingot Casting Process: Fionn Iversen[1]; Jon Arne Bakken[1]; Stein Tore Johansen[1]; [1]Norwegian Institute of Science and Technology (NTNU), Matls. Tech. & Electrochem., A. Getz vei 2B, Trondheim N-7491 Norway

In conventional direct chill (DC) hot-top casting of aluminium extrusion ingot using 'gas-slip', poor surface quality of the cast ingot may appear. It is believed that these defects are related to instabilities such as periodic oscillations or folding of the meniscus (the interface between liquid metal and gas in the mould). The object of this work is to develop a stable and reliable model for simulation of the meniscus dynamics. A new 2D cylinder symmetric front tracking model has been developed for the meniscus propagation, and is implemented in a general Navier Stokes

solver. The model is based on a finite volume cubic spline marker chain technique. The advantages of the model is its applicability to cases with large density ratios and its ability to calculate independent velocity fields for phases on separate sides of an interface, thereby making it possible to model the dynamics of thin films with a thickness scale smaller than the typical grid size. Effects of surface tension and wetting are also easily applied in the marker chain model. The model is applied to the DC casting process. Results are compared with data from plant test runs and suggestions are made on how to improve the casting process.

3:10 PM

Computational Modeling of Heat Mass and Solute Transport in Directional Solidification Processes: Mohammed El Ganaoui[1]; Patrick Bontoux[2]; [1]Université de Limoges, Phys./Numcl. Mod., 123 Albert Thomas, Limoges 87000 France; [2]CNRS, Numcl. Mod., IRPHE, Marseille, 13451 France

During directional solidification, absorption or rejection of latent heat or solute by the solidification front induce convective flows in the liquid phase. These convective motions affect heat and mass transfer in the vicinity of the solidification interface and is subject to many studies. In this work a numerical approach is presented. To avoid remeshing needed by front tracking methods a time-dependent homogeneous formulation is considered to verify implicitly thermal and solutal Stefan conditions at the interface. The numerical solution is based on finite volume approximation. The previous work show that the present method describe accurately the hydrodynamic transition and the interaction with the solid liquid interface in the case of pure material. This study focuses on the occurrence of solutal convection in gradient freezing applications. In a first step only the fluid phase is investigated and the results are validated with respect to spectral ones. In a second step the full solid/liquid model is investigated. A linear approximation of the equilibrium phase diagram is considered for establishing relations between mass fraction and temperature fields to close the set of conservation equations. The present work shows that the method is able to describe with accuracy close to spectral one complex phenomena occurring in reduced configuration to fluid phase. The global model with solid phase account correctly the interface displacement and its interaction with solutal field.

3:35 PM Break

3:50 PM

Computational Modelling of Freeze Layers in Smelting Processes: Andrew P. Campbell[1]; Koulis A. Pericleous[1]; Mark Cross[1]; [1]University of Greenwich, Ctr. for Numl. Modlg. & Proc. Analy., 30 Park Row, Greenwich, London SE10 9LS UK

The use of computational modelling in examining process engineering issues is very powerful. It has been used in the development of the HIsmelt® process from its concept. It is desirable to further water-cool the HIsmelt® vessel to reduce downtime for replacing refractory. Water-cooled elements close to a metal bath run the risk of failure. This generally occurs when a process perturbation causes the freeze and refractory layers to come away from the water-cooled element, which is then exposed to liquid metal. The element fails as they are unable to remove all the heat. Modelling of the water-cooled element involves modelling the heat transfer, fluid flow, stress and solidification for a localised section of the reaction vessel. The complex interaction between the liquid slag and the refractory applied to the outside of the water-cooled element is also being examined to model the wear of this layer. The model is being constructed in Physica, a CFD code developed at the University of Greenwich. Modelling of this system has commenced with modelling solidification test cases. These test cases have been used to validate the CFD code's capability to model the solidification in this system. A model to track the penetration of slag into refractory has also been developed and tested.

4:15 PM

Mathematical Modeling of Heat Transfer and Microporosity Formation in Die Cast A356 Wheels: P. Vo[1]; D. Maijer[1]; S. L. Cockcroft[1]; M. A. Wells[1]; C. Hermesmann[2]; [1]University of British Columbia, Dept. of Metals & Matls. Eng., Vancouver, British Columbia V6T 1Z4, Canada; [2]Canadian Autoparts Toyota, Inc., 7233 Progress Way, Delta, British Columbia V4G 1E7, Canada

Die cast aluminum wheels are one of the most difficult automotive castings to produce because of stringent cast surface and internal quality requirements. A mathematical model has been developed to predict heat transport and porosity formation in die cast A356 wheels as part of a collaborative research agreement between researchers at the University of British Columbia and Canadian Auto Parts Toyota Incorporated. The heat transfer model, employing the commercial finite element code ABAQUS, is a three-dimensional, 30° slice of the wheel and die that describes forced air cooling, natural convection of the die to the surrounding environment, and interfacial heat transport between the wheel and die sections. Extensive temperature measurements in the die and in the wheel taken over several cycles in the casting process were used to fine tune and validate the model. Preliminary work on predicting porosity formation focused on using the Niyama parameter as a measure of the probability of porosity. The latest version of the model incorporates a new more fundamentally based porosity criterion, which takes into account the effect of hydrogen and inclusion content. The development of this model together with some early results will be presented.

4:40 PM

Modelling Filters in Metal Casting Processes: Mark R. Jolly[1]; Jean-Christophe Gebelin[1]; [1]The University of Birmingham, IRC in Matls., Edgbaston, Birmingham, W. Midlands B15 2TT UK

A number of different types of so-called filters are used on the metal casting industries to impart some cleaning effect and flow control on the liquid metal as it passes through them. The filters range from simple planar meshes through extruded channels to reticulated foam structures. It is most common that software packages used in the industry model the filters by a simple pressure drop associated with some area fraction and permeability parameters. Recent experimental work at the IRC in Birmingham has shown that filters of the same type can behave very differ-

ently depending upon the casting process in which they are employed. Modelling filter geometries for a range of different casting processes has indicated that the flow of metal and heat losses through the filters are rather complex and should be considered when using filters in the casting processes. This paper will present a number of cases of different types of filters modeled and different processes and indicate some of the sensitivities of the processes to boundary conditions imposed by the process.

5:05 PM
Computer Heat Transfer Model for Directionally Solidified Castings: Deming Wang[1]; R. A. Overfelt[1]; [1]Auburn University, Mechl. Eng. Dept., 201 Ross Hall, Auburn University, AL 36849 USA

Thermal transfer control is very important in directionally solidified (DS) castings. This paper presents a simple and efficient computer-aided heat transfer simulation method to predict the thermal characteristics of an alloy sample in a special furnace for directional solidification. A two-dimensional transient heat transfer by radiation combined with conduction is developed to calculate the energy exchange between the symmetric furnace and the sample. A control volume technique is used to obtain a set of highly efficient finite difference equations for heat conduction and heat radiation with changeable view factors. The model well simulates the transient process of DS castings. The simulation results are verified by a few measurable experimental results. Using the two-dimensional computer simulation model, many thermal properties of the samples can be obtained, such as temperature distribution, solidification velocity, the shapes and positions of the liquid/solid interface and thermal gradient at the interfaces. These are very important to analyze microstructure of DS casting alloy, avoid casting defects and control the quality of DS castings.

Tuesday AM Plenary Session
9:00 AM–9:45 AM

Tuesday AM — Room: St. Tropez/Monte Carlo
September 25, 2001 — Location: Hilton San Diego Resort

Session Chair: James W. Evans, University of California, Dept. of Matls. Sci. & Min. Eng., 585 Evans Hall, Berkeley, CA 94720-1760 USA

Keynote
Phase Field Methods for Modeling Microstructure: James A. Warren[1]; [1]National Institute of Standards and Technology, Metall. Div. & Ctr. for Theoretl. & Computl. Matl. Sci., Gaithersburg, MD 20899 USA

The phase field method has been successfully employed as both a tool to model heterogeneous materials and as numerical method for calculating the motion of interfaces and phase boundaries without explicitly tracking those interfaces. The method has been used to model a diverse suite of problems describing the microstructural evolution in materials. These models are derived from thermodynamic arguments and symmetry principles, and usually guarantee positive local entropy production for systems out of equilibrium. Descriptions of how phase field methods can be applied to the problems of solidification, grain growth, and electroplating will be presented.

Track A - Structure

Tuesday AM — Room: St. Tropez
September 25, 2001 — Location: Hilton San Diego Resort

Session Chair: Jim Warren, NIST, CTCMS & Metall. Div., Gaithersburg, MD 20899-8554 USA

9:45 AM
Microporosity Evolution and Interdendritic Fluid Flows during Solidification: Adrian S. Sabau[1]; Srinath Viswanathan[1]; [1]Oak Ridge National Laboratory, Matls. & Cer. Div., Bldg. 4508, MS 6083, Oak Ridge, TN 37831 USA

The occurrence of microporosity during metal casting is due to the combined effects of solidification shrinkage and gas precipitation. The governing equations for fluid flow and hydrogen evolution indicate that porosity formation and fluid flow are strongly coupled. However, in most studies on microporosity, it is considered that the porosity formation does not influence the fluid flow in the mushy zone. In this study, a computational methodology is presented for the numerical simulation of microporosity evolution and interdendritic fluid flow. The solution algorithm presented includes a fully coupled, implicit treatment of microporosity and local pressure in the mushy zone. It is shown that neglecting the effect of porosity formation on the pressure in the mushy zone yields higher pressure drops and an over-prediction of final porosity. By its growth, microporosity compensates partially for the solidification shrinkage, reducing the feeding demand. Therefore, in order to accurately describe casting defects, comprehensive models of fluid flow, heat transfer, solidification, must include the effect of microporosity as well.

10:10 AM
Cellular Automata Computer Model of Polycrystalline Plastic Deformation: Alexander V. Spuskanyuk[1]; Yakiv E. Beygelzimer[1]; Victor M. Varyukhin[1]; [1]Donetsk Physical & Technical Institute of the NAS of Ukraine, High Press. Phys. & Adv. Tech. Dept., 72 R. Luxembourg St., Donetsk 83114 Ukraine

Effects stipulated by interdependence of microlevel and macrolevel of plastic deformation processes were analyzed. Using computing mechanics instead of constitutive relationships the adequate computer models were used, which was opened by cellular automata approach. By means of numerical experiments, the cellular automata allowed to study the macrobehavior of the ensemble of cells at the macrolevel depending on the local microscopic laws that define evolution of each cell and its interaction with the closest environment. A cellular model of the plastic deformation of polycrystalline aggregate was proposed and comprehensively described. Representative volume of the deformed solid body deformed was described as a population of interconnected units which, in turn, consisted of

lower scale level units. Sliding along the various allowed sliding systems deforms simple units, which do not have an internal structure. For consideration of stress distribution within the limits of components, the approach of self-consistent field was used. Rotation of units and moment stresses connected with it were taken into account. Results of computer experiments are analyzed, software is described.

10:35 AM Break

10:50 AM
Simulations of Microstructural Evolution: Martin E. Glicksman[1]; Kegang Wang[1]; P. Crawford[1]; [1]Rensselaer Polytechnic Institute (CII-9111), Matls. Sci. & Eng., 110 8th St., Troy, NY 12180-3590 USA

Predicting microstructure evolution in alloys remains a keystone of materials science. The mean-field theory of phase coarsening, in the (impractical) limit of zero volume fraction, was first formulated by Lifshitz and Slyozov, and by Wagner (LSW). Numerous attempts have been made to extend LSW theory toward microstructures with nonzero volume fractions. The successes achieved with analytical theories, however, have been limited, due primarily to the difficulties of characterizing interactions among particles and the matrix, and accounting for stochastic variations in the microstructural locale surrounding each particle. Such theories predict unrealistic particle size distributions (PSDs) when compared with experimental observations. The importance of large-scale simulation of microstructures was realized with concurrently increasing capability of computer hardware and software. Since the 1980s we formulated and solved multiparticle diffusion equations to simulate the dynamics of phase coarsening. These simulations provide insight into the nature of diffusion interactions and multiparticle stochastics. The rate constants, PSDs, and higher-order correlations can all be extracted by simulation. "Snap shot" simulation techniques, developed recently permit study of microstructure size at various volume fractions. Gradually, a bridge has been built connecting fundamental theory and experiment through computer simulations. Some recent examples of progress in simulating microstructure evolution will be discussed.

11:15 AM
Ab Initio Calculations of Theoretical Tensile Strength in Metals and Intermetallics: Mojmir Sob[1]; Ligen Wang[1]; Martin Friak[1]; Vaclav Vitek[2]; [1]Institute of Physics of Materials, Zizkova 22, Brno 616 62 Czech Republic; [2]University of Pennsylvania, Dept. of MSE, 3231 Walnut St., Philadelphia, PA 19104-6272 USA

Fully self-consistent ab initio electronic structure calculations of the theoretical tensile strength in metals and intermetallics loaded uniaxially along several crystallographic directions are performed using the full-potential LAPW method. It turns out that the theoretical tensile strength and elastic anisotropy at higher strains are closely connected with the presence or absence of higher-symmetry structures along corresponding deformation paths. Total energy calculations show that all higher-energy cubic structures studied are locally unstable with respect to tetragonal and/or trigonal deformation modes. In intermetallics, there may or may not be symmetry-dictated energy extrema corresponding to cubic lattices depending on the atomic ordering. However, other energy extrema along the deformation paths besides those required by symmetry occur. Configurations corresponding to energy minima on the deformation paths may represent metastable structures that can play an important role in interfaces and other extended defects. As a specific example, tensile strength of single-crystalline tungsten loaded uniaxially along the [001] and [111] directions is analyzed. Although tungsten is elastically nearly isotropic for small deformations theoretical tensile strength exhibits a marked anisotropy. This anisotropy is explained in terms of structural energy diferences between bcc, fcc and simple cubic structures which occur on the calculated deformation paths. Theoretical results compare favorably with available experimental value obtained for tungsten whiskers grown along the [110] direction. Further examples include computer simulations of a tensile test for single-crystalline NiAl, where the theoretical tensile strength for the "hard" orientation [001] differs very significantly from that for the [111] orientation. Again, this anisotropy may be understood in terms of higher-symmetry structures present or absent along the deformation paths.

11:40 AM
Modeling of Interdendritic Strain and Interden-dritic Cracking Phenomena during Dendritic Solidification Processes: Mostafa El-Bealy[1]; [1]Material Processing International, 100 Trade Centre Dr., #103, Champaign, IL 61820 USA

A one-dimensional mathematical model to calculate the interdendritic cracking tendencies for low alloyed carbon steel casting processes is described. The model combines an interdendritic strain model with concept of the effect of alloying element on the solidification behaviour, segregation of carbon, and therefore, critical elementary interdendritic area EIA. A susceptibility of cracking of different steels is modelled by using El-Bealy approach. Model predictions were performed to explain the effects of various alloying elements on the solidification and cracking phenomena. Some typical cases in conventional casting processes related to increase cracking susceptibility are discussed. It is shown that there is a satisfactory degree of correlation between prediction a practical casting knowledge. Possible solutions to these problems based on the adjustment of chemical composition are proposed.

Track B - Melting & Solidification - II

Tuesday AM
September 25, 2001

Room: Portofino/Marseilles
Location: Hilton San Diego Resort

Session Chairs: Dan Cook, Virginia Commonwealth University, Mechl. Eng. Dept., 601 W. Main St., Rm. 312, Box 843015, Richmond, VA 23284-3015 USA; Mark Jolly, University of Birmingham, Birmingham, Great Britain B15 2TT UK

9:45 AM
Wax Injection in the Investment Casting Industry: Jean-Christophe Gebelin[1]; Alexander Cendrowicz[1]; Mark R.

Jolly[1]; [1]The University of Birmingham, IRC in Matls., Edgbaston, Birmingham, W. Midlands B15 2TT UK

Injection of wax patterns is the first stage of the multi-stage process of investment casting. The quality of the final casting and its dimensional accuracy is highly dependent on this stage of the process. Pattern waxes used in the industry behave in a complex visco-elastic-plastic manner. The modelling of such material behaviour is therefore not simple. In this paper a number of configurations of die will be shown in which the injection of the wax has been carried out for a range of processing conditions. Some of the dies are transparent and the movements of wax front observed can be compared with those predicted by simulation. Surface defects in final components will also be shown and compared with the location predicted by simulation software. Some discussion will be presented on the limitations of the software used and the time-scales achieved for practical use as a design tool within the foundry environment.

10:10 AM

Micro/Macro Modeling of Ingot Cooling Processes for Ni-Cu-S Alloys: Apostle Mouchmov[1]; Mark Cross[1]; Koulis Pericleous[1]; [1]University of Greenwich, Sch. of Compg. & Mathl. Sci., 30 Park Row, Greenwich, London SE10 9LS UK

Copper–nickel–sulphide alloys are typically cooled and solidified in 4, 8 and 16 tonne ingots. These ingots exhibit a variation of grain size distribution and macro segregation of the prime alloy components throughout. The former is assumed to be primarily due to the dominant relation between grain growth rate and the cooling profile, whilst the latter is heavily influenced by buoyancy driven residual convection. The objective of this research program is to examine the extent to which it is possible to develop a 'broad brush' computational model of this ingot cooling process, that can predict some 'integral' measure of the grain size (e.g. average diameter) and the macro-segregation as a function of operating conditions. A computational modeling software framework, PHYSICA+ is used to simulate the complex process of ingot casting, which involves coupling between different physical phenomena. The entire model involves: (i) a 'broad brush' grain growth model that could be used in the prediction of micro/macro-structure of alloy ingot cooling processes, (ii) a heat transfer and solidification model which takes into account a second phase transformation of Ni3S2 to heazle-woodite, and (iii) NS fluid flow simulation which provides a good basis for further micro/macro segregation modeling. At this stage some results of the 3D convection driven thermal cooling and solidification profiles will be shown, together with the 'integral' model for the grain size prediction.

10:35 AM Break

10:50 AM

Comparison of Numerical Models of Solidification Behavior in Direct Chill Casting with Experiments: Christopher J. Vreeman[2]; David Schloz[3]; Matthew John M. Krane[1]; [1]Purdue University, Sch. of Matls. Eng., W. Lafayette, IN 47907 USA; [2]Boeing North American, Rocketdyne Div., 6633 Canoga Ave., Canoga Park, CA 91309 USA; [3]Wagstaff, Inc., 3910 N. Flora Rd., Spokane, WA 99216 USA

Numerical results from a continuum mixture model of the Direct Chill casting process is compared to experimental results from industrial scale aluminum billets. The model, which includes the transport of free-floating solid particles, is used to simulate the effect of a grain refiner on macroseg-regation and fluid flow. It is applied to an Al-6wt%Cu alloy and the effect of casting speed, grain refiner, and assumed mushy zone permeability on predicted macrosegregation, sump profile, and temperature fields are presented. Three 45 cm diameter billets were cast under production conditions with and without grain refiner and at two casting speeds. Temperature and composition measurements and sump profiles are compared to the numerical results. The comparison shows qualitative agreement and limitations of application of the model to industrial processes are discussed.

11:15 AM

Two-Phase Predictive Finite-Element Flow Model for Semi-Solid Slurries: Frédéric Pineau[1]; [1]National Research Council Canada, Indl. Matls. Inst., Proc. Modlg. & Instrm., 75 de Mortagne Blvd., Boucherville, Québec J4B 6Y4 Canada

Semisolid metal alloys have a special microstructure of globular grains suspended in a liquid metal matrix. This particular physical state of the matter can be exploited to produce near-net-shape parts with improved mechanical properties. However, the behavior of the slurry is strongly influenced by the local solid fraction and state of agglomeration. Different flow instabilities associated with the combined flow and solidification process result, which make difficult the application of semisolid processing in the casting industry. Moreover, the rheology of semisolid materials is not well understood. Most of the theory has been derived from experimental data, which are somewhat difficult to measure. A model that accounts for the multiphase nature of the slurry is required to get more insight into such complex flows. This paper thus describes a mixture model for semisolid slurries. It assumes that the mixture of liquid-solid components behaves as a single fluid as far as overall mass and momentum balances are concerned. The coupling force between the phases is derived on the assumption that the slurry is a fluid saturated isotropic media. The proposed methodology is implemented in a finite element code. The filling of an industrial-scale capillary flow viscometer is investigated numerically. Segregation patterns are obtained and discussed.

11:40 AM

CFD Simulation of Continuous Charging and Melting of Small Metallic Particles in a Melting Reactor: Stefan Pirker[1]; Oszkar Biro[3]; Philipp Gittler[1]; Peter Mittag[2]; Bernard Aigner[2]; [1]Johannes Kepler University, Altenbergerstr. 69, Linz A-4040 Austria; [2]VOEST ALPINE Industrieanlagenbau GmbH, Postfach 3, Linz A-4031 Austria; [3]Technical University Graz, Kopernikusgasse 24, 8010 Graz, Austria

This paper considers CFD modelling of processing and melting of small metallic particles by means of electrical heating. The particles fall continuously onto a liquid metal bath which is heated by an electric arc. After melting of the particles liquid metal is tapped. The charging behavior of the particles in the supply unit as well as in the reactor freeboard is studied by means of Euler-Euler granular simulations. The flow situation in the metal bath due to gas injection and magnetic fields is calculated by combining

Navier-Stokes and Maxwell solvers. The macroscopic melting process occurring during the continuous charging of the particles is studied by kinetic laws for melting reactions. The temperature field is evaluated by balancing heat sources due to Joule's heating and heat losses due to latent heat of melting as well as convection and radiation. As a result of these simulations the fully three-dimensional flow fields of particles and gas in the atmosphere is obtained. Furthermore the flow field as well as the magnetic field in the metal bath can be studied. As a main result the three-dimensional concentration field of the still unsolved particles in the liquid metal can be evaluated.

12:05 PM
Numerical Simulation of Wax Pattern Dimensions in Investment Casting: Adrian S. Sabau[1]; Srinath Viswanathan[1]; [1]Oak Ridge National Laboratory, Matls. & Cer. Div., Bldg. 4508, MS 6083, Oak Ridge, TN 37831 USA

Dimensional Changes between a pattern die and its corresponding investment cast part occur as a result of complex phenomena such as thermal expansion/contraction and hot deformation (elastic, plastic, and creep) during the processing of the pattern material (wax), mold material (shell), and solidifying alloy. Determining the pattern tooling dimensions is crucial to the dimensional control of the investment casting process. To date, there are no computational methodologies available for predicting dimensional changes during investment casting. This paper deals with the evaluation of wax pattern dimensions, which is one important factor in determining the pattern tooling dimensions in investment casting. Cerita 29-51, an industrial wax is considered in this study. The wax pattern dimensions are affected by its thermophysical and thermomechanical properties, restraint of geometrical features by the metal die, and process parameters such as dwell time, platen temperature, injection pressure and injection temperature. Numerical simulation results for the wax pattern dimensions are compared with experimental measurements. Critical variables that determine dimensional changes associated with the wax system are identified.

Tuesday PM Plenary Session
2:00 PM–2:45 PM

Tuesday PM
September 25, 2001
Room: St. Tropez/Monte Carlo
Location: Hilton San Diego Resort

Session Chair: Koulis Pericleous, University of Greenwich, Greenwich Maritime Campus, Greenwich, London SE10 9LS UK

Keynote
Computational Modelling of Metals Reduction Processes: Phil Schwarz[1]; [1]CSIRO Minerals, Box 312, Clayton S., Victoria 3163 Australia

This paper reviews the status of computational modelling of a variety of common metals reduction processes, namely the blast furnace, rotary kiln and fluidised bed, and one new process not yet commercialised, namely smelting-reduction as in the HIsmelt® Process. In each case, the last decade has seen the emergence of the capability to simulate the processes using multi-phase reacting computational fluid dynamics techniques. In some cases this capability is still in the process of being developed, and the next few years will see the maturing of the modelling techniques. As they become established, it will be possible to apply them to further refine the older technologies such as blast furnaces and rotary kilns, and assist in the optimisation, commercialisation and acceptance of the newer technologies such as fluidised bed and molten bath reduction. The development of a computational fluid dynamic model of bath smelting-reduction is described in some detail to illustrate how a large number of complex and interacting phenomena can be successfully simulated within a CFD framework.

Track A - CFD Modelling - II

Tuesday PM
September 25, 2001
Room: St. Tropez
Location: Hilton San Diego Resort

Session Chairs: Phil Schwarz, CSIRO Minerals, Box 312, Clayton S., Victoria 3163 Australia; Pascal Gardin, IRSID, Maizieres-les-Metz France

2:45 PM
Modelling of Raceway Hysteresis: Govind S. Gupta[1]; S. Sarkar[1]; M. G. Basavaraj[1]; P. D. Patil[2]; [1]Indian Institute of Science, Dept. of Metall., Bangalore 560 012 India; [2]Indian Institute of Science, Dept. of Cheml. Eng., Bangalore 560 012 India

Previous experimental study on raceway size hysteresis on two-dimensional cold model showed that the interparticle and wall-particle friction had a very large effect on the raceway size. Existing literature correlations for raceway size ignore the frictional effects. It has also been shown in the present study that their applicability to the ironmaking blast furnace is questionable. To take into account the effect of friction on the raceway size a stress analysis has been done for the raceway region. The partial differential equations for the stresses have been developed and solved computationally. The frictional forces were obtained in terms of stresses. To predict the raceway size a force balance was done for the raceway zone considering the pressure force, the frictional force and the bed weight. The resulting equations from the force balance are able to describe the raceway hysteresis phenomena correctly along with the raceway size. A two dimensional experimental set up has been fabricated in order to validate the computer predictions. Predicted values agree well with the experimental values. A correlation has been developed to predict the raceway size.

3:10 PM
Lifetime Prediction of Pneumatic Conveyor Bends with the Aid of Computational Models: Mayur K. Patel[1]; Robert Hanson[1]; [1]University of Greenwich, Ctr. for Numl. Modlg. & Proc. Analy., 30 Park Row, Greenwich SE10 9LS UK

The puncture of pneumatic conveyor bends in industry causes several problems. Two important factors are: (1) Escape of the conveyed product causing health and dust

hazard and (2) Repairing and cleaning up after punctures necessitates shutting down conveyors, which will affect the operation of the plant, thus reducing profitability. Bends in pneumatic conveying systems tend to wear out and puncture first since particles generally strike the bend walls with larger intensity than straight pipe sections. Current models for bend lifetime prediction are inaccurate as they fail to account for key parameters that are of fundamental importance to the progression of the wear. The provision of an accurate predictive method would lead to improvements in the structure of the planned maintenance programmes, thus reducing unplanned shutdowns. The paper reports the first phase of a study undertaken to develop and implement a CFD based engineering tool to predict the lifetime of conveyor bends for two- and three-dimensional test cases. The model used is based on Eulerian and Lagrangian methods. It is unique in that the erosion due to the particle impacts is accounted for within a CFD framework, thus taking into account angle of attack and impact velocity, ensuring more realistic predictions of the wear profile and their grid dependency and sensitivity to the inlet particle distributions.

3:35 PM Break

3:50 PM
A Parametric Study of Oxy-Fuel Burners in Secondary Aluminum Melting: Madhu Huggahalli[1]; Neeraj Saxena[1]; Ken Grieshaber[2]; Jerry Bernardski[2]; David Stoffel[2]; [1]BOC Gases, Tech., 100 Mountain Ave., Murray Hill, NJ 07974 USA; [2]BOC Gases, 575 Mountain Ave., Murray Hill, NJ 07974 USA

The use of oxy-fuel burners in secondary aluminum melting applications offers several advantages including reduced fuel consumption, faster charge to tap times and lower NOx emissions. Their successful, safe and economical use in a furnace depends on several factors and considerations such as burner and flue placement, metal circulation, charge practices and the type of refractory used in the furnace. These factors required in the successful conversion of furnaces from air-fuel to oxy-fuel based burners are discussed in detail in this paper. Critical parameters are identified and examined using computational fluid dynamics (CFD) simulations. Parameters are estimated via laboratory testing and validated through trials performed at commercial installations. Guidelines and a simplified approach to estimate à priori the economic impact of converting from air-fuel to oxy-fuel are presented. The final products of this research are simplified and validated tools for modeling aluminum furnaces. These include improved heat and energy balance models and parameterized CFD solutions which allow rapid customization to individual furnace configurations. These tools provide field engineers with immediate and accurate predictions of performance, allowing for repeated precise scenario analyses.

4:15 PM
Computational Modelling of Vortex Formation in the Lead Refining Kettle: Suman Kumar[1]; Chris Bailey[1]; Mayur Patel[1]; A. W. Piper[2]; M. Cowling[2]; R. A. Forsdick[2]; [1]University of Greenwich, 30 Park Row, Greenwich, SE10 9LS UK; [2]Britannia Refined Metals, Ltd., Northfleet, UK

The refining of lead bullion takes place in hemispherical vessels (known as kettles) of various sizes. It is normal practice to remove impurity elements (i.e. copper, silver, bismuth, antimony, etc.) sequentially, by the addition of reagents. This process has been in operation for many years in refineries all over the world. Unfortunately very little is understood about the actual mixing and refining process taking place in these kettles. This paper will present a detailed modelling analysis of this process, where computational and physical modelling techniques have been used. The computational fluid dynamics (CFD) techniques used to model fluid mixing by impellers will be discussed and results will be presented comparing CFD data with plant data. Also discussed will be the modelling techniques used to simulate the reactions taking place in the vessel during impurity removal.

4:40 PM
CFD Modeling of Solids Suspensions in Stirred Tanks: Lanre Oshinowo[1]; André Bakker[2]; [1]Hatch, 2800 Speakman Dr., Mississauga, Ontario L5K 2R7 Canada; [2]Fluent, Inc., 10 Cavendish Ct., Lebanon, NH 03766 USA

Mechanical agitation is widely used in process industry operations involving solid-liquid flows. The typical process requirement is for the solid phase to be suspended for the purpose of dissolution, reaction, or to provide feed uniformity. If these vessels are not functioning properly, by inadequately maintaining suspension, the quality of the products being generated can suffer. Associated with the operation of these units is a need to maintain the suspension at the lowest possible cost. The challenge is in understanding the fluid dynamics in the vessel and relating this knowledge to design. CFD modeling can provide insight to both the multiphase transport and the design parameters. An understanding of the parameters that govern the just-suspended impeller speed, Njs, and the distribution of solids, is critical. Recent advances in computational fluid dynamics allow for the modeling of multiphase systems, such as the liquid-solid mixtures discussed here. Of particular interest is the Eulerian multiphase model, which uses separate sets of Navier-Stokes equations for the liquid and solids (or granular) phases. Incorporating moving impeller modeling techniques, such as, the sliding mesh method, provides a rigorous estimate of the solids suspension behavior. This paper will assess the current design parameter Njs in the context of scale-up and compare it to the quality of solids dispersion as a means of assessing correct scale-up in suspension tank design. The work presented includes a study of a 45° pitched-blade turbine and a hydrofoil impeller. Both single and dual impeller operation have been evaluated. For a given impeller style in a fixed vessel, D/T and C/T are varied to explore suspension flow patterns at Njs. The settled solids fraction for speeds below Njs, and the cloud height for impeller speeds above Njs were studied. The CFD results correspond well with experimental literature data on velocity distribution and cloud height.

5:05 PM
Water Model and Numerical Study on the Spout Height in a Gas Stirred Vessel: Diancai Guo[1]; G. A. Irons[1]; [1]McMaster University, Steel Rsrch. Ctr., 1280 Main St., Hamilton, Ontario L8S 4L7 Canada

The average spout height and width produced by bottom gas injection in a water model of a steel ladle were

measured with an image processing technique. It was revealed that the spout height could be described by a Gaussian curve. A combined SIMPLE-VOF model was developed to simulate the liquid surface and flow. The results showed that, though the model produced reasonable velocity distributions and free surface positions, the spout height due to the dynamic head of the rising liquid was substantially lower than observed, indicating that the bubble dynamics at the bath surface play an important role in spout height.

Track B - Thermo-Mechanical Modelling - I

Tuesday PM
September 25, 2001

Room: Portofino/Marseilles
Location: Hilton San Diego Resort

Session Chairs: Brian G. Thomas, University of Illinois–Urbana, Dept. of Mechl. & Indl. Eng., Urbana, IL 61801 USA; Danny Wheeler, NIST, Gaithersburg, MD 20899-8555 USA

2:45 PM

Thick Yield Surface: An Approach to the Processing of Computer Experiments on Polycrystalline Deformation: Yan E. Beygelzimer[1]; Alexander V. Spuskanyuk[1]; Victor Varyukhin[1]; [1]Donetsk Physical & Technical Institute of the NAS of Ukraine, High Press. Phys. & Adv. Tech. Dept., 72 R. Luxembourg St., Donetsk 83114 Ukraine

The main idea of the report is that the yield surface can be presented as thick, "foamed surface" with dimensionality exceeding two. By other words, perhaps, the yield surface is fractal, i.e. it belongs to the geometric objects with fractional dimensionality. Apparently, fractal structure of the yield surface is determined by the fractal structure of natural materials. Besides, the "cloud of internal stresses" term is introduced to describe the stress distribution in RVE. Its plastic flow is determined by the interaction of this cloud with the thick yield surface. Thick yield surface and internal stress cloud concepts allow to determine the additional correlation between micromechanical models of polycrystals and phenomenological theory of plasticity.

3:10 PM

Model for Stress, Temperature and Phase Transformation Behaviour of Steels on Run-Out Table in Hot Strip Mill: Heung Nam Han[1]; Jae Kon Lee[1]; Hong Jun Kim[1]; Young-Sool Jin[1]; [1]Pohang Iron & Steel Co., Ltd. (POSCO), Sheet Prod. & Rsrch. Grp., Techl. Rsrch. Labs., Pohang PO Box 36, 1 Koedong-dong, Nam-ku, Pohang-shi, Kyungbuk 790-785 Korea

A mathematical model was developed considering non-symmetric cooling and stress distribution in both thickness and width direction of strip on a run-out table of hot strip mill. In order to solve a transient heat transfer equation including the heat evolved from phase transformation, a finite difference method coupled with thermodynamic and kinetic analyses was applied. The heat capacity of each phase and heat evolution due to phase transformation were obtained from the thermodynamic analysis of the Fe-C-Mn-Si system based on a sublattice model. The phase transformation kinetics of the steels was derived by using continuous cooling experiments and the thermodynamic analysis. Heat transfer coefficients of strips on the run-out table were, by applying an inverse method, determined from actual mill data under various cooling conditions. As for the stress analysis, the density change of strip due to cooling and phase transformation and the transformation induced plasticity were considered. A constitutive equation for the transformation induced plasticity, which is related to the phase transformation kinetics and the applied stress, was newly suggested. A finite element method was adopted to calculate the deformation behaviour of strip on run-out table.

3:35 PM Break

3:50 PM

Thermo-Mechanical Coupling Finite Element Analysis of Sheet Metal Extrusion Process: Zhanghua Chen[1]; C. Y. Tang[1]; T. C. Lee[1]; [1]The Hong Kong Polytechnic University, Dept. of Mfg. Eng., Hung Hom, Hong Kong, China

In sheet metal forming process, the forming limit and strain distribution are governed by plastic instability and fracture following strain localization. It has been proved that the temperature gradient caused by plastic deformation, heat transfer, and friction between sheet and tools is one of crucial factors to induce the strain localization in high speed metal forming processes. In this paper, a numerical simulation of the sheet metal extrusion process has been conducted by using thermal-mechanical coupling finite element method. In the investigation, the sheet metal extrusion is assumed to be a non-isothermal and elasto-plastic process. The material of workpiece is SS400 steel which is the same as that used in experiment. The boundary energy dissipation due to heat convection has been taken into account. Bishop's step-wise decoupled strategy is adopted to handle coupling between mechanical deformation and the temperature variation. This technique has been proven to be robust and efficient for large thermal-plastic deformation computation. By adopting this approach only the pure mechanical parts of the weak forms have to be consistently linearized since the coupling terms are held constant during the iteration. In order to avoid locking deficiency that frequently exhibited in classical displace-based finite element method, an improved large deformation mixed finite element method has been used to solve this near-incompressible metal forming problem. The standard Newton-Raphson iteration method together with the corresponding consistent tangent operator has been adopted to solve nonlinear algorithmic equations. In thermal phase, the transient heat transfer finite element method together with the Crank-Nicholson algorithm has been employed to determine the temperature field. The total time for extrusion process is specified to be 0.4 second. Using the numerical result, the effect of temperature distribution on forming limit is discussed. By comparing with the experimental result, it has been revealed that the temperature gradient plays an important role to induce the strain localization and lead to fracture failure in metal material.

4:15 PM

A Model for Calculating the Lankford Value in Sheet Steels: Sihai Jiao[1]; C. Isaac Garcia[2]; Anthony J. DeArdo[2]; [1]Shanghai Baosteel Group Co., Shanghai Baosteel Rsrch.

Inst. (R&D Ctr.), 1 Kedong Rd., Baoshan Dist., Shanghai 201900 China; [2]University of Pittsburgh, Basic Metals Proc. Rsrch. Inst., Matls. Sci. & Eng. Dept., 848 Benedum Hall, Pittsburgh, PA 15261 USA

The deep drawing capacity of sheet steels is generally indicated by the Lankford value, which is mainly determined by the texture in steels. Traditionally, various models derived from the Taylor model are employed to calculate the Lankford value from the texture. Due to the complexity of the texture description, the current models could be quite difficult to use and, moreover, a considerable error may be caused by the incompletion of including some trivial texture components. The present work proposes a practical model based on the Hill Equation to calculate the Lankford Value of interstitial free (IF) steels, by considering only a few selected texture components. In IF steels, a new parameter describing texture, the Texture Intensity Ratio (TIR), i.e. (111)/(100), not only affects the average Lankford value, but also has a strong influence on its distribution. By using the new TIR parameter, the texture based prediction models can be used more easily to calculate the Lankford value. The distribution of the Lankford value as function of the angle with respect to the rolling direction seems to be influenced by Mn and P additions. The practical significance of the results from this work will be presented and discussed.

4:40 PM

Interfacial Modelling of Hot Rolling: A Probabilistic Approach: Sumitesh Das[1]; Eric J. Palmiere[1]; Ian C. Howard[2]; [1]The University of Sheffield, Dept. of Eng. Matls., Sir Robert Hadfield Bldg., Mappin St., Sheffield, S. Yorkshire S1 2JD UK; [2]The University of Sheffield, Dept. of Mechl. Eng., Sir Frederick Mappin Bldg., Mappin St., Sheffield, S. Yorkshire S1 2JD UK

Heat transfer and friction in hot flat rolling have traditionally been characterised by an average heat transfer coefficient (h) and an average friction coefficient (μ). However, the presence of oxide scales and asperities at the interface question the use of such averages. The apparent irregularity and lack of pattern of interactions at the interface has prompted this present investigation to move away from averaged h and μ values, and to study their local evolution based on probabilistic rules. The approach is based on the probability of finding the workpiece surface in a specific configuration at a particular instance of time in the roll gap. These rules are based on observations of surface phenomena such as scale behaviour during hot rolling. The model is implemented using user-subroutines integrated with the commercially available finite element program ABAQUS. The results show the strong dependence of h and μ on the local scale interactions. In particular, the effect of scale thickness, material behaviour and processing conditions on the evolution of h and μ are discussed. Finally, the development of a Cellular Automata based Finite Element (CAFE) model is proposed to model the combined interfacial phenomenon of friction and heat transfer at the tool-work piece interface.

5:05 PM

Computational Experiment in the Mechanics of Materials: Leon Mishnaevsky[1]; Ulrich Weber[1]; Nils Lippmann[2]; Siegfried Schmauder[1]; [1]University of Stuttgart, Staatliche Materialprüfungsanstalt (MPA), Pfaffenwaldring 32, D-70569 Stuttgart, Germany; [2]Robert Bosch GmbH, FV/PLM, PO Box 300240, D-70442 Stuttgart, Germany

A computational approach to the optimization of fracture resistance of multiphase materials (here-high speed steels) by varying their microstructure is presented. The main points of the optimization of steels are as follows: (1) development and verification of the model: numerical simulation of crack initiation and growth in real microstructures of steels, (2) computational experiment: simulation of crack growth in different idealized quasi-real microstructures and (3) the comparison of fracture resistances of different microstructures and the development of recommendations to the improvement of the fracture toughness of steels. Numerical simulations of crack growth in real microstructures of steels and different idealized carbide distributions are carried out. On the basis of the simulations, recommendations for the improvement of high speed steel microstructures are given. It is shown that the fracture resistance of the steels is much higher for the fine than for the coarse version of the same type of microstructures.

Wednesday AM Plenary Session
9:00 AM–9:45 AM

Wednesday AM — Room: St. Tropez/Monte Carlo
September 26, 2001 — Location: Hilton San Diego Resort

Session Chair: Mark Samonds, UES Software, Inc., 175 Admiral Cochran Dr., Annapolis, MD 21401 USA

Keynote

Micro-Macro Modeling of Solidification Processes and Phenomena: Vaughan Voller[1]; [1]University of Minnesota, 500 Pillisbury Dr., Minneapolis, MN 55455 USA

The wide range of length and time scales found in solidification processes are outlined and discussed. Methods for Direct Microstructure Simulation (DMS) are introduced. Key features in sharp interface and phase field models are presented. Concepts in micro-macro solidification modeling are covered. Basic details of microstructure and segregation models are provided. A description of a recent segregation micro-macro model is presented in detail.

Track A - Heat & Mass Transfer - II

Wednesday AM — Room: St. Tropez
September 26, 2001 — Location: Hilton San Diego Resort

Session Chairs: Tom Battle, DuPont Company, White Pigment & Min. Prod., Edgemoor, DE 19809 USA; Rod Guthrie, McGill Metals Processing Center, Montreal, Quebec H3A 2B2 Canada

9:45 AM

A Steady State Electrothermic Simulation Analysis of a Carbothermic Reduction Reactor for the Production of

Aluminium: Dimitrios I. Gerogiorgis[1]; B. Erik Ydstie[1]; Sridhar S. Seetharaman[2]; [1]Carnegie Mellon University, Dept. of Cheml. Eng., 5000 Forbes Ave., Pittsburgh, PA 15213 USA; [2]Carnegie Mellon University, Dept. of Matls. Sci. & Eng., 5000 Forbes Ave., Pittsburgh, PA 15213 USA

Carbothermic reduction is an important process alternative for aluminium production, based on the endothermic chemical reduction reaction occurring between aluminium oxide and carbon. This process has potential for drastic reduction of fixed and operational costs of the investment. Furthermore, it is environmentally benign and in principle significantly more energy-efficient, as the costly electrolytic ionization is effectively avoided by direct chemical reduction. Carbon monoxide production can contribute to the energy integration of the process, as the installation of a conjugate power cycle allows for production of electric energy necessary for heating purposes. The carbothermic production of aluminium can occur in a two-stage high-temperature reactor. Carbon and aluminium oxide pellets are introduced into an electric arc furnace (1st stage) and undergo melting at a temperature of ca. 1950°C, thus forming a high-temperature molten slag. This multicomponent molten slag (carbon, aluminium oxide and carbide, carbon monoxide) is fed to a subsequent 2nd stage, where it reacts at a higher temperature (2050°C) to aluminium. The 2nd stage reaction products (carbon monoxide, molten pure aluminium) are then separated. The present study focuses on a Computational Fluid Dynamics (CFD) simulation of the flowfield within the carbothermic reduction reactor, which is an essential step for the effective conceptual design of pilot and production plants. This CFD simulation of the melt flow encompasses important research challenges, due to the limited knowledge of thermo-physical properties for high-temperature multicomponent molten slags and the significant experimental limitations. The computational domain for the CFD simulation is defined as a rectangular sector, while the computational expense of the simulation can be minimized by considering symmetry planes. The CFD model for computation adopts simplifying assumptions for production (Joule effect) and consumption (endothermic reaction) of heat, considering a pseudohomogeneous molten slag. The CFD simulation is performed in a hexahedral structured grid (selecting uniform meshing) using a commercially available CFD code (CFX 4.3-AEA) with some necessary modifications. The main objective of the present CFD simulation study is to extract conclusions regarding the design of a carbothermic reactor and also understand how process parameters affect this system.

10:10 AM

The Limitations of CFD Modelling for Furnace Atmosphere Troubleshooting: Paul F. Stratton[1]; Neeraj Saxena[2]; M. Huggahalli[2]; [1]BOC Gases, European Dvlp. Ctr., Rother Valley Way, Holbrook, Sheffield, SY S20 3RP UK; [2]BOC Gases R&D, 100 Mountain Ave., Murray Hill, NJ, USA

Furnace temperatures and atmospheres are the most important factors in an industrial heat treating processes. To create an atmosphere in a continuous furnace, several gases, either singly or as mixtures, are used. These include nitrogen, hydrogen, exothermic and endothermic atmospheres, natural gas, propane and cracked methanol. Which gas or gases and how much of each should be used in the furnace is largely based on experience or on expensive trial and error experiments. BOC Gases has developed a simplified, easy-to-use PC based model to facilitate the understanding, troubleshooting and design of atmosphere injection into heat treating furnaces and to minimise wasteful experimentation. The model takes into account the role of oxygen, nitrogen, hydrogen, methane, carbon monoxide, carbon dioxide and water vapour in the heat treating process. Fundamental energy and mass conservation equations are solved to determine atmosphere profiles in a furnace for given compositions of gases injected. The reducing and carburising potentials of the gases, necessary to design any heat treating process, can be deduced using this model. The model can also be used to design and troubleshoot the atmosphere injection practice. Using model simulations, the critical process variables can be identified and the heat treating process optimised using a minimal number of experiments on the production floor. To validate the model industrial examples are examined. The results of this model were found to compare quite well with actual data obtained from production furnaces.

10:35 AM Break

10:50 AM

Simulation of Internal Oxidation: Henrik Larsson[1]; Martin Schwind[1]; John Ågren[1]; [1]Royal Institute of Technology, Matls. Sci. & Eng., Stockholm SE-100 44 Sweden

Internal oxidation is simulated in three dimensions using a combined random walk-cellular automata approach. Nucleation theory is used for the early stages of growth. Diffusion is modelled utilising discrete units, whereby a transformed Fick-Onsager law is solved by a simple stochastic method. Growth and dissolution of precipitates are treated by applying the local equilibrium hypothesis and the Gibbs-Thomson equation. Grain boundaries are included in the model; their effect on diffusion, nucleation and growth are taken into account.

11:15 AM

Dynamic Model for a Vapor Recovery in Carbo-thermic Aluminum Process: Vianey Garcia-Osorio[1]; Tor Lindstad[2]; B. Erik Ydstie[1]; [1]Carnegie Mellon University, Cheml. Eng., 5000 Forbes Ave., Pittsburgh, PA 15213 USA; [2]SINTEF, Matls. Tech., Alfred Getz vei 2, Trondheim N-7465 Norway

As a result of the high temperatures present in a Carbothermic Aluminum Process the content of aluminum and aluminum sub oxide in the gases leaving this process is high. These gases must be recovered. For this purpose a Vapor Recovery Unit is introduced in the system. Inside this unit the aluminum compounds react in a series of heterogeneous non-catalytic reactions forming solid, liquid and gas products. The different product phases depend on the temperature present in the system. Therefore the model needs to capture the physics of the system and accurately represents the interaction between the energy and material balances and process thermodynamics. In this work a dynamic model of the Vapor Recovery Unit is presented. Because of the complexity of the system several models are developed and coupled to capture the essential physics of the multiphase reaction problem. A shrinking core model is used to describe the reaction mechanisms. Then material and energy balances are coupled with the thermodynamic properties from the FACT database of physical properties,

resulting in a system of nonlinear Partial Differential Equations. In the paper we describe the model development and governing equations for the reaction mechanisms and fluid flow. Finally we review the numerical schemes created for the solution of the model system. The model can be used for control and design purposes.

11:40 AM
Computer Simulation of the Structure-Energetical Transformations at Combustion Synthesis in the Systems NiAl and TiAl: Mikhail D. Starostenkov[1]; Gennadiy M. Poletayev[1]; Alexandra S. Starostenkova[1]; [1]Altai State Technical University, Gen. Phys. Dept., 46 Lenina Pr., Barnaul, Altai Region 656099 Russia

It is known, that combustion synthesis (CS) takes place at high velocities. That is why it is difficult to determine the stages of structure-energetical transformations, taking place at CS. The process of CS is modelled by the computer simulation, using molecular dynamics method. The investigating systems are presented in a form of bimetal thin films at the beginning of the process. The interactions between the atoms are given by the sets of emperic pair potentials. The set of critical parameters, regulating the velocity of the reaction of CS is found in the result of computer experiment. The parameters are the following: limited free volume, its connection with the temperature of the process beginning, the velocity of components mixing, the velocity of formation of intermetallic phases. It is established, that the structure transformations of the system take place at the formation of nanocrystal phases in the process of CS. Character of structure-energetical transformation at combustion synthesis in the systems NiAl and TiAl depend from the orientation of contacting plains in bimetal thin films.

12:05 PM
Influence of Surface Pressure and Slag Layer on Bubble Bursting in Degasser Systems: Julie Cranga[1]; Pascal Gardin[1]; Didier Huin[1]; Jacques Magnaudet[2]; [1]IRSID, THEMEF, Voie Romaine, BP30320, Maizieres les Metz 57283 France; [2]IMFT, Groupe Interface, Allee du Professeur Camille Soula, Toulouse 31400 France

For the control of steel grade in steelmaking reactors, IRSID and IMFT are building a new modelling of bubble behavior in the vicinity of liquid steel/slag interface. The objective is to identify the main parameters affecting hydrodynamics of the different phases and to supply the mass transfer models commonly used at IRSID with the appropriate fluid mechanic parameters (local velocities, bubble residence time in the melt ...). Special emphasis is given to the study of pressure influence on bubble bursting. The topics of the paper are: *First to describe the numerical VOF method developed to predict the multiphase flow including bubbles, liquid metal and slag layer. *Second to analyze the influence of pressure in RH degasser on bubble bursting. Validation is given by comparison with previous results in literature. The major point concerns the distinct behavior whether the pressure is low or high. *Third to study the influence of slag layer on liquid metal entrainment in the wake of the bubble and on the nature of projection from the bath surface, in relation with the slag layer thickness and physical properties (viscosity and interfacial tension).

Track B - Melting & Solidification - III

Wednesday AM
September 26, 2001

Room: Portofino/Marseilles
Location: Hilton San Diego Resort

Session Chairs: Mark Samonds, UES Software, Inc., 175 Admiral Cochran Dr., Annapolis, MD 21401 USA; Srinath Viswanathan, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6083 USA

9:45 AM
Computational Studies of the Control of Convection in Diamagnetic Liquids during Solidification with Magnetic Field Gradient: C. B. Seybert[1]; J. W. Evans[1]; [1]University of California, Dept. of Matls. Sci. & Eng., Berkeley, CA 94720 USA

Natural convection is a commonplace phenomenon in the solidification of materials. Driven by temperature gradients, concentration gradients or both, it plays a role in the development of macrosegregation and the microstructure of the solid. The paper describes an investigation, both by experiment and by mathematical modeling, into this natural convection and whether it can be controlled by the application of a magnetic body force. This force is not the Lorenz force, that can be used to damp convection in conducting fluids, but the magnetic body force that arises from a gradient in the magnetic field. If that gradient is of the right size and direction it can be made to eliminate buoyancy or even to levitate a fluid. The experimental investigation has entailed the measurement of velocities and solidification front positions in transparent liquids, with PIV used for the former. The measurements have been carried out for water and aqueous solutions of manganese chloride. In the latter case most of the measurements have been made with the solution in the bore of a superconducting magnet at Marshall Space Flight Center and it has been demonstrated that natural convection in this paramagnetic solution can be greatly reduced, perhaps halted, by the magnetic field. Measurements agree reasonably well with computations performed using FLUENT and this CFD package has been used to predict the conditions under which natural convection within a diamagnetic fluid might be halted.

10:10 AM
Methods for Approximating Discontinuous or Rapidly Changing Conductivity in Numerical Calculations: Vaughan Richard Voller[1]; [1]University of Minnesota, Civ. Eng., 500 Pillsbury Dr. S.E., Minneapolis, MN 55455 USA

Much is said in the recent literature on the modeling necessity of obtaining appropriate thermo-physical properties; in particular the requirement to account for properties that are "strong" functions of the depended variables, e.g., temperature. Of course obtaining appropriate thermophysical properties serves no purpose unless they can be accurately integrated into a discrete numerical calculation. The purpose of this paper is to examine how temperature dependent conductivities that exhibit discontinuities or

rapid changes can be handled in a numerical code. A simple approach based on a local application of a Kirchoff transformation at the discrete level is presented. The application of this transformation–that does not require any inversion–is demonstrated on solving a range of one and two dimensional test problems.

10:35 AM Break

10:50 AM
Modelling of the De-Waxing of Investment Cast Shells: Jean-Christophe Gebelin[1]; Sam Jones[1]; Mark R. Jolly[1]; [1]The University of Birmingham, IRC in Matls., Edgbaston, Birmingham, W. Midlands B15 2TT UK

The de-waxing process in investment casting is truly a black art which is carried out in a black hole–the autoclave. The process involves exposing wax, coated by a porous ceramic shell, to steam at a pressure of 10 bar and a temperature of about 180°C. The process which then occur are truly multi-media and multi-physics. Steam condenses in the porous ceramic, wax melts and flows, the shells expand and sometimes crack. Why the shells crack is one of the most difficult questions asked in the industry. Modelling and validating the de-waxing process is not simple. The IRC at the University of Birmingham is attempting to model this process using Physica+ a code developed in the UK. This paper will present the latest results in the attempt to model one of the casting industries most intractable problems.

11:15 AM
The Swirling Effect in an Immersion Nozzle on the Flow in a Continuous Casting Mold: Shinichiro Yokoya[1]; Sigeo Takagi[1]; Manabu Iguchi[1]; Katsukiyo Marukawa[3]; Shigeta Hara[2]; [1]Nippon Institute of Technology, Mechl. Eng., 4-1 Miyashiro, Minami-saitama, Saitama 345-8501 Japan; [2]Osaka University, Dept. of Matls. Sci. & Proc., Yamadaoka, Suita, Osakafu 565-0000, Japan; [3]Osaka University, Sumitomo Metal Industries, Ltd., Japan

A numerical analysis and water model study of the mold region of a continuous casting apparatus are performed with a novel injection concept using swirling flow in the pouring tube, to control the heat and mass transfer in the continuous casting mold. As a result, the following results were found: (1)By changing swirl strength, it is easy to control the flow pattern as well as the direction of the flow. (2)Uniform velocity distribution can be obtained within a very short distance from the outlet of the nozzle. (3)Heat and mass transfer near the meniscus can be remarkably activated compared with a conventional straight type immersion nozzle without swirl. (4)Swirl helps the superheat in the melt dissipate. (5)Penetration depth of the nozzle outlet flow is decreased remarkably by the application of swirling. Those findings mentioned above are very useful to control the flow pattern in the continuous caster.

11:40 AM
Computational Modelling of Metals Extrusion and Forging Processes: A. J. Williams[1]; T. N. Croft[1]; M. Cross[1]; [1]University of Greenwich, Ctr. for Numl. Modlg. & Proc. Analy., The Old Royal Naval College, 30 Park Row, London SE10 9LS UK

The computational modelling of extrusion and forging processes is now well established. In this work a novel approach is described which utilises finite volume methods on unstructured meshes. This technique can be used to solve simultaneously for fluid flow, heat transfer and nonlinear solid mechanics and their interactions. The approach involves the solution of free surface non-Newtonian fluid flow equations in an Eulerian context to track the behaviour of the workpiece and its extrusion/forging, and the solution of the solid mechanics equations in the Lagrangian context to predict the deformation/stress behaviour of the die. Some preliminary examples of this approach will be discussed.

12:05 PM
The Role of Orifice Shape in the Detection of Inclusions in Liquid Metals: Roderick I.L. Guthrie[1]; Mei Li[1]; [1]McGill Metals Processing Centre, Canada

A mathematical model was developed to study the role of orifice shape in the detection of inclusions in LiMCA (Liquid Metal Cleanliness Analyzer) system. The fluid flow field within the ESZ was obtained by solving the Navier-Stokes equations. The trajectories of entrained particles were calculated using the equations for motion of particles. A numerical study of the effect of orifice shape on signal shape generated by inclusions passing through orifice showed that the signals in a parabolic orifice are gaussian in shape, while those in a cylindrical orifice are trapezoidal in shape. This signal shape difference needs to be taken into account when performing particle discrimination. Orifice shape influences also pass-through fraction of inclusions. Finally, a study of the orifice shape on critical conditioning currents suggested that as the polynominal coefficient of the parabolic orifice increases, the critical conditioning current, which is also the maximum operating current, decreases dramatically. These critical conditioning currents also increase as the fluid flow velocity within the ESZ increases.

Wednesday PM Plenary Session
2:00 PM–2:45 PM

Wednesday PM
September 26, 2001

Room: St. Tropez/Monte Carlo
Location: Hilton San Diego Resort

Session Chair: Brian G. Thomas, University of Illinois–Urbana, Dept. of Mechl. & Indl. Eng., Urbana, IL 61801 USA

Keynote
Computational Modeling of Thermo-Mechanical Phenomena: Christopher Bailey[1]; [1]University of Greenwich, 30 Park Row, Greenwich, London SE10 9LS UK

Many industrial processes involve materials that are subject to temperature change and thermal stress. Examples range from the casting of large metallic products to the cooling and reliability of small electronic components. Thermally induced stress is a major concern as it can lead to material damage and product failure. Material properties, thermal and mechanical, and process conditions such as the size and location of a feeder in metals casting, or the power dissipation in a computer chip, will govern the magnitude of these stresses. Temperature may also be influ-

enced by fluid flow, for example, the airflow over a computer chip in a laptop will govern the rate of heat extraction, hence the temperature gradients in the chip and the evolving thermal stresses. This paper provides details on the governing equations for heat transfer (temperature) and solid mechanics (stress), their degree of coupling, and the numerical techniques used to solve them. Three examples are discussed to illustrate the use thermomechanical modelling. These also provide an insight into the degree of coupling required between the equations. The first example, involves thermal cycling of electronic components where a prescribed temperature field is applied. As temperature is known, this example only requires the solution of the stress equation. The second example also involves the modelling of an electronic component where the temperature field is also calculated. In both of these examples, the stress calculation is dependent on the temperature field, but the temperature calculation is not dependent of the solution of the stress equation (one-way coupling). The final example provides details on modelling the metals casting process. Both the temperature and stress equations are solved but, unlike the previous two examples, in this case the temperature field is dependent on the results from the stress calculation (two-way coupling).

Thermo-Mechanical Modelling - II

Wednesday PM Room: St. Tropez
September 26, 2001 Location: Hilton San Diego Resort

Session Chairs: Chris Bailey, University of Greenwich, 30 Park Row, Greenwich SE10 9LS UK; Brian G. Thomas, University of Illinois–Urbana, Dept. of Mechl. & Indl. Eng., Urbana, IL 61801 USA

2:45 PM
Mathematical Modeling of Mean Flow Stress during Hot Strip Rolling of Nb Microalloyed Steels: Ki Bong Kang[1]; Sang Hyun Cho[2]; John J. Jonas[2]; [1]POSCO, Rsrch. Lab., 1 Goedong-dong Nam-gu, Pohang, Kyungbuk 790-785 S. Korea; [2]McGill University, Dept. of Metall. Eng., 3610 University St., Montreal, Quebec H3A 2B2 Canada

The recrystallization behavior of Nb microallyed steels was studied using hot torsion testing with the aim of modeling the recrystallization processes taking place hot rolling. It is shown that the recrystallization kinetics depend on steel composition and processing conditions. The stress-strain curves were determined in order to derive new equations for the peak stress, peak strain, mean flow stress and softening kinetics. The peak strain is influenced by the presence of alloying element; their addition, which has a solute effect, retards the rate of grain boundary motion, shifting the peak to the right. The addition of Ni to the steel results in a significant increment in the activation energy for hot deformation, but Cr has the opposite effect. It was also found that the deformation activation energy in these steels was not altered by the addition of Mo and Nb. The kinetics of static and metadynamic recrystallization were characterized and appropriate expressions were formulated for the recrystallization kinetics. The rate of metadynamic recrystallization increases with strain rate and temperature and is observed to be independent of strain, in contrast to the observation for static recrystallization.

3:10 PM
Modeling of Residual Stresses and Mechanical Behavior of Glass-Infiltrated Spinel Ceramic Composites: Anil Saigal[1]; Edwin R. Fuller[2]; Said Jahanmir[2]; [1]Tufts University, Mechl. Eng., 200 College Ave., Medford, MA 02155 USA; [2]National Institute of Standards and Technology, Cer. Div., Bldg. 223, Gaithersburg, MD 20899 USA

All-ceramic crowns, including glass-infiltrated alumina and spinel composites, are coming into widespread use because of their superior aesthetics and chemical inertness. This study investigates the residual stresses that are developed in these composites as a result of cooldown from the glass-infiltration temperature to room temperature due to slight mismatch in the coefficients of thermal expansion and its effect on the mechanical behavior of these composites. Two-dimensional finite element simulations were performed using an object oriented finite element program OOF. The OOF program is a combination of two programs. The first program, PPM2OOF, is designed to read an image file such as a micrograph. The individual pixels that constitute the micrograph may be collected into groups and their material properties assigned. PPM2OOF is then used to create the finite element model/mesh that OOF then reads. The average residual stresses are found to be tensile in the alumina and spinel matrix and compressive in the infiltrated-glass. There is large variation in residual stresses and strains from location to location with presence of locations at which the glass is under tensile stress. The crack initiation and initial propagation in glass-spinel composites is at the glass-spinel interface in both the glass and the spinel. The presence of residual stresses can lead to lower crack initiation stresses and degrade the mechanical properties of the composites.

3:35 PM Break

3:50 PM
Simulation of Fatigue Stress Life (S-N) Diagrams for Ti-6Al-4V Alloy by Application of Artificial Neural Network: S. McShane[1]; Savko Malinov[1]; J. J. McKeown[1]; Wei Sha[1]; [1]The Queens University of Belfast, Sch. of Civ. Eng., Belfast, Northern Ireland BT7 1NN UK

A model is developed for prediction of fatigue stress life S-N diagrams for Ti-6Al-4V alloy at different conditions, using Artificial Neural Network (ANN). Different factors which have influence on the S-N diagram are involved as input parameters of the NN, namely microstructure, environment, texture, test/work temperature, surface treatment and stress amplitude. As the output the S-N fatigue diagram is simulated and plotted. The model is based on standard multilayer feed forward neural network. The NN is trained with a comprehensive data set collected from the literature, using Levenberg-Marquardt training algorithm in combination with Bayesian regularisation. A very good performance of the trained Neural Network is achieved. Good correspondence between ANN prediction and experimental S-N diagrams is observed. Using the model S-N diagrams for different conditions are predicted and analysed. Graphical User Interface is developed for use of the model. We believe that the model will be important for

practical applications in solving various problems on fatigue behaviour of the titanium alloy.

4:15 PM
Prediction of Lateral and Normal Force-Displacement Curves for Flip-Chip Solder Joints: Daniel Wheeler[1]; Daniel Josell[1]; James A. Warren[1]; William E. Wallace[1]; [1]National Institute of Standards and Technology, Metall. Div., 100 Bureau Dr., MS 8555, Gaithersburg, MD 20899-8555 USA

We present the results of experiments and modeling of flip-chip geometry solder joint shapes under shear loading. Modeling, using Surface Evolver, included development of techniques that use an applied vector force (normal and shear loading) as input to determine a vector displacement of the pads connected by the solder joint (standoff height and misalignment). Previous solutions solved the converse problem: fixed displacements used to determine required applied force. Such solutions were inconvenient for applications, where the applied force (chip weight) is known. Also, for geometric and materials studies of solder joint shapes involving multiple parameters, determining the equilibrium displacement from applied force by bracketing solutions could become computationally expensive. Measurements of solder joint standoff height and misalignment as functions of the applied force (normal and shear), solder volume and pad diameter are presented. Experiments were carried out for solder ball diameters from 15 mil (0.029 mm^3 volume) to 6 mil (0.0019 mm^3 volume) on pads of diameter 0.64 mm and 0.35 mm. Fitting of simulation to experimental results gave optimised values for the contact angle and surface tension of the solder which were consistent with measured and literature values.

4:40 PM
Simulation of the Plastic Behavior during Mechanical Testing of Galvanized Steel using the Finite Element Method: Adriana Salas[1]; Martha Patricia Guerrero Mata[1]; Rafael Colás[1]; René Garza[2]; [1]Universidad Autonoma de Nuevo Leon, FIME-Programa Doctoral en Materiales, Cd. Universitaria, San Nicolas de los Garza, Nuevo Leon 66450 Mexico; [2]Galvak, SA de CV, Quality Assurance, Ave. de la Juventud 340 Nte, Col Cuauhtemoc, San Nicolas de los Garza, Nuevo Leon 66450 Mexico

The use of the finite element method (FEM) for studying the plastic behavior of the metals has become a common practice over the few past years, because it has been proved to be a good means of evaluating processes parameters, and predicting and improving the processes, avoiding the traditional trial and error technique. FEM was used via a commercial package (Ansys) to create a three dimensional model to simulate tension uniaxial simple tests for a galvanized low carbon steel. The aim of the work was to analyze the plastic behavior of a distribution of grains on the zinc cover of a set of galvanized low carbon steel samples. The samples were drawn a mesh with lines 2 mm apart on one of their faces. The samples were deformed at room temperature, at constant low crosshead speed, stopping deformation at different times. Before and during the stops of the testing the deformation measurements were recorded for further calculations in an image analyzer in order to compare these with the computational predictions, as well as validate the numerical model. The results of this study can be extended to other testing conditions, besides the model can used for obtaining constitutive equations.