Process Control and Optimization in Ferrous and Non Ferrous Industry: Plenary, Thermodynamics and Bio-Processing

Sponsored by: Extraction & Processing Division, Materials Processing & Manufacturing Division, Jt. MPMD/EPD-Process Modeling Analysis & Control Committee, EPD-Pyrometallurgy Committee

Program Organizers: Florian Kongoli, FLOGEN Technologies, Inc., Materials Technology Department, Montreal, Quebec H3S 2CS Canada; Matthew John M. Krane, Purdue University, Department of Materials Engineering, West Lafayette, IN 47907 USA; Luis Ruiz-Aparicio, University of Pittsburgh, Pittsburgh, PA 15261 USA; Krich Sawamiphakdi, The Timken Company, R&D Manufacturing Technology, Canton, OH 44706 USA; Brian G. Thomas, University of Illinois, Department of Mechanical and Industrial Engineering, Urbana, IL 61801 USA

Monday AM Room: Regency Ballroom D
November 10, 2003 Location: Hyatt Regency Downtown Hotel

Session Chairs: Florian Kongoli, FLOGEN Technologies Inc., Matls. Tech. Dept., Montreal, QC H3S 2C3 Canada; Brian G. Thomas, University of Illinois, Mechl. & Industl. Engrg. Dept., Urbana, IL 61801 USA

8:00 AM Florian Kongoli: Opening Remarks

8:10 AM Plenary

New Opportunities in Optimization and Control of Metals Processing: H. Shang[1]; J. B. Wiskel[2]; J. F. Forbes[2]; *H. Henein*[2]; [1]Laurentian University, Sch. of Engrg., Sudbury, ON P3E 2C6 Canada; [2]University of Alberta, Dept. of Chem. & Matls. Engrg., Edmonton, AB T6G 2G6 Canada

The materials science and metallurgical engineering communities have expended enormous resources in developing high fidelity process models. Exploiting such deep knowledge of these processes for Model-based Optimization (MBO) and Model Predictive Control (MPC) is a new frontier in materials process engineering that will exploit state-of-the-art models and lead to exceptional process performance. This paper will begin with a short survey of the development and availability of high quality process models within the literature and a discussion of how these could be used to improve process operation. A summary of the current "state-of-the-art" in process automation technologies and the conventional framework in which these technologies are deployed will be presented. An illustration of the use of MBO in process design and operations will be presented for the continuous casting of steel. In addition, a simple run-out table simulation will be used to demonstrate the power of the MPC technique.

8:35 AM Plenary

Interactions of Molten Fe-Cr Alloy with Refractories: Yuhsuke Mizukami[1]; Tsuneo Itoh[2]; Masakazu Kimoto[3]; Takahiro Miki[4]; Tetsuya Nagasaka[4]; *Mitsutaka Hino*[4]; [1]Tohoku University, Grad. Sch. of Engrg., Aoba-yama 04, Sendai 980-8579 Japan; [2]Shibukawa Works, Daido Steel Co. Ltd., Formerly of Tohoku University; [3]Hitachi Systems and Services Ltd., Formerly of Tohoku University; [4]Tohoku University, Dept. of Metall., Grad. Sch. of Engrg., 02 Aoba-yama, Sendai 980-8579 Japan

Crude high Cr containing steel such as tool steel, heat-resistant steel or stainless steel is produced by dissolution of high carbon ferro-chromium into molten crude steel. In the refining process, decarburization is performed at the first stage, and deoxidation is followed in the next stage. Therefore, the equilibrium relation between dissolved Cr and O in molten Fe-Cr alloy after decarburization is very important when yield of deoxidizer is considered for the overall control and optimization of the process. It is well known that the yield of deoxidizer does strongly depend on the kinds of refractories of furnace in the secondary refining process. In the present work, the equilibrium relation between dissolved Cr and O in molten Fe-Cr alloy has been measured in a Cr_2O_3, MgO or Al_2O_3 crucible at steelmaking temperature. O contents at given Fe-Cr components have been lower in order of Cr_2O_3, Al_2O_3 and MgO crucible. The present results have been discussed based on the activities of the constituents in pure solid Cr_2O_3, and $FeO.Cr_2O_3$, $MgO.Cr_2O_3$ and $(Al,Cr)_2O_3$ solid solutions.

9:00 AM Plenary

On-Line Detection of Quality Problems in Continuous Casting of Steel: *B. G. Thomas*[1]; [1]University of Illinois, Dept. of Mechl. & Industl. Engrg., 1206 W. Green St., Urbana, IL 61801 USA

Quality problems can be identified as they occur by monitoring mold signals (level sensor, thermocouples in the mold walls, friction) and taking appropriate action (such as slowing casting speed, changing taper, changing a clogged nozzle, or later visual inspection of the surface for possible downgrading. Surface depressions and groups of deep oscillation marks form at meniscus and reduce local heat transfer as they move down the mold at the casting speed. This slows shell growth, increases shell surface temperature, and causes characteristic dips in mold thermocouple signals. More importantly, they are associated with longitudinal cracks. Characteristic thermocouple signatures have been identified for many defects, including sticker breakouts, transverse depressions and deep oscillation marks, narrow-face bleeds, transverse corner cracks, longitudinal cracks, flux entrapment from mold level fluctuation, and other problems. With the help of computational models, these mold signals should be used to troubleshoot defects, and to take appropriate corrective action.

9:25 AM Plenary

Process Control, Optimization and Automation Through Modeling and Simulation: *Florian Kongoli*[1]; Ian McBow[1]; S. Llubani[1]; [1]FLOGEN Technologies Inc., Metals Dept., 5757 Decelles Ave., Ste. 511, Montreal, QC H3S 2C3 Canada

Nonferrous and ferrous smelting industries have recently faced the unavoidable necessity of changing and/or improving the smelting technologies as a result of the use of new raw materials which are becoming available from different geographical areas. These new feed materials usually contain different ore composition and higher level of minor components, which adversely affect the smelting process. Due to the problems encountered in several processes as a result of this feed diversification some work has been undertaken in order to make uniform the feed and avoid later surprises in the smelting process. However this has proven to be very difficult and sometimes almost impossible. In this work a more viable approach is undertaken to deal with this problem. It consists of controlling not the cause of the problem i.e. the feed composition but instead the results of this feed change, i.e. the end-point of smelting technologies. It is shown that this approach, when carried out through advances thermophysicochemical modeling and simulation tools is not only easier and less costly but it also helps the control optimization and automation of the smelting processes. Several examples are given and future work is underlined.

9:50 AM Break

10:00 AM Invited

Effects of Ca Addition on the Thermodynamic Properties of P and B in Molten Silicon Alloys: *Kazuki Morita*[1]; [1]The University of Tokyo, Dept. of Matls. Engrg., 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656 Japan

A new route to produce solar grade silicon (SOG-Si 6N) from metallurgical grade (MG-Si 98%) has been developed in Japan, which may satisfy the increasing demand of solar cells in the near future. Since some elements such as P and B have very large distribution coefficients, they cannot be removed by solidification refinings and electron beam vacuum refining and oxidation plasma refining should be conducted, which leads to higher energy cost. In our previous research the leaching procedure with Ca addition was found to be very effective for Fe and Ti removal because of calcium silicide formation in which Fe and Ti were concentrated. At the same time P and/or B could be removed if their affinities for Ca are large. In the present research the effects of Ca addition on the thermodynamic properties of P and B in molten silicon alloys have been investigated for proper control and optimization of the overall process. The interaction parameters between Ca and P, and Ca and B were determined by chemical equilibration techniques at 1723 K. Although the interaction parameter between Ca and B was rather small, that between Ca and P showed a large negative value. Also, the results for the leaching test with various amount of Ca addition revealed that the removal ratio of both elements, especially P, drastically increased with the increase in the Ca content, which showed very good agreement with the prediction from the interaction parameters derived in the present work. The present results suggest that the preliminary leaching procedure can reduce the processing time and energy for SOG-Si refining.

10:25 AM Invited

Experimental Techniques to Characterize High-Temperatures Processes Such as the Direct Decomposition of Metal Sulfides: *Marcel Sturzenegger*[1]; I. Alxneit[1]; C. Guesdon[1]; M. Musella[1]; H.-R. Tschudi[1]; L. Winkel[1]; [1]Paul Scherrer Institut, High-Temp. Solar Tech., OVGA/103, 5232 Villigen PSI Switzerland

Though the extraction of copper is well established, generation of sulfur dioxide (SO2) is still a troublesome issue. Conventional processes are further challenged by the increasing amount of impurities in the concentrates. Direct decomposition of the metal sulfides into the metal(s) and elemental sulfur under concentrated solar radiation offers a promising path to solve both problems. Thermogravimetric measurements under inert atmospheres have shown that synthetic chalcocite or chalcopyrite yield copper at temperatures as low as 1773 K. Even though optimum reaction temperatures might be somewhat higher, such temperatures are straightforwardly accessible in solar chemical reactors. The absence of oxygen will reduce the extent of slag forming reactions and thereby alter the evaporation characteristics of volatile impurities such as arsenic or antimony. Chemical equilibrium calculations for a chalcopyrite-enargite feed, e.g., have shown that under inert atmospheres arsenic compounds are completely evaporated at temperatures above 1000 K and an effective separation of arsenic from the matte is expected. An important step towards a solar production of copper is the design and testing of prototype solar chemical reactors for this reaction. Numerical modeling is a key tool supporting a rational design but it requires data of the high-temperature properties that prevail in these processes. Development of techniques for determining the essential quantities such as decomposition rates or radiative properties at temperatures up to 2000 K is therefore a main activity in our laboratory in order to control and optimize the process. Though developed in the frame of high-temperature solar technology, the experimental techniques are also suited to advance the understanding of conventional high-temperature processes.

10:50 AM Invited

Thermodynamic Simulation of Complex Metallurgical and Chemical Systems With the Method of Chemical Dynamics: *B. Zilbergleyt*[1]; *M. Zinigrad*[2]; [1]System Dynamics Research Foundation, Chicago, IL USA; [2]College of Judea and Samaria, Ariel Israel

Current understanding of the chemical equilibrium is based exclusively on the probabilistic considerations that are correct for isolated systems with only one chemical reaction to take place. For the systems with multiple chemical interactions, current thermodynamics promotes the idea of openness, artificially flavored with coefficients of thermodynamic activity. Recently introduced thermodynamics of chemical systems and the Method of Chemical Dynamics (MCD) offer explicit accounting for the multiple chemical interactions within the system. In the new theory, thermodynamic equilibrium of the j-subsystem obeys the logistic equation DGj/RT - tjDj(1-Dj)=0, (1) rigorously derived from the currently recognized concepts of thermodynamics. Having the only new parameter - the subsystem's reduced chaotic temperature tj to describe external interactions, and reaction extent Dj as the independent parameter, this equation covers the whole domain of the system's possible states - from true thermodynamic equilibrium through the open equilibrium to bifurcations and chaos depending on the tj value. The MCD brings new opportunities to thermodynamic simulation and optimization of complex metallurgical and chemical systems, allowing for the analysis of their domains of states and the area limits, and for more accurate calculations of the equilibrium composition. Its usage is exemplified by several applications like reactions between the Co and Ni double oxides with sulfur, natural gas combustion, some others.

11:15 AM Invited

Parameters for Control and Optimisation of Bioleaching of Sulphide Minerals: *H. Deveci*[1]; *A. Akcil*[2]; I. Alp[1]; [1]Karadeniz Teknik Universitesi, Dept. of Mining Engrg., Trabzon TR 61080 Turkey; [2]S. Demirel University, BIOMIN Grp., Mineral Procg. Div., Dept. of Mining Engrg., Isparta TR 32260 Turkey

Bioleaching/biooxidation is essentially a dissolution process with the involvement of acidophilic bacteria acting as the “catalyst” to accelerate the dissolution of metals from sulphide minerals. The contribution of bacteria to the metal dissolution is closely controlled by the growth of bacteria, which is itself affected by the physico-chemical conditions within the bioleaching environment. There are a number of operating parameters controlling bioleaching processes, which are required to be maintained within a certain range in the leaching environment whereby the activity of bacteria with the resultant oxidation of sulphide minerals can be optimised. In this regard temperature, acidity, oxidising conditions, availability of nutrients, oxygen and carbon dioxide, surface area and presence of toxic ions are of prime importance for control and optimisation of bioleaching of sulphide ores/concentrates. Bioleaching processes are temperature and pH dependent with optimum metal dissolution occurring in a particular range where the bacterial strain is most active e.g. mesophiles at 35-40°C and pH 1.6-2.0. Provision of nutrient salts is required to maintain the optimum growth and hence metal dissolution with the quantity of nutrients apparently being dependent on the availability of substrate i.e. head grade/pulp density of an ore/concentrate. Oxygen transfer is one of the most critical factors since the oxygen levels below 1-2 mg/l may adversely affect the oxidising activity of bacteria. In the bioleaching environment oxidising conditions should be maintained by bacteria to efficiently dissolve the sulphide minerals, e.g. >400 mV vs Ag/AgCl for ZnS. Bioleaching rate tends to improve with increasing the surface area at low pulp densities but, in practice, the pulp density is limited to ~20% w/v. Increasing concentrations of ions such as Cl- may also adversely affect the oxidative activity of bacteria.

11:40 AM Invited

Investigation of Genus Alyssum Species for Control and Optimization of Nickel Phytoextraction Processes and Phytoremediation of Nickel Contaminated Soils: *A. Hasko*[1]; A. Çullaj[2]; F. Kongoli[3]; [1]Agricultural University of Tirana, Dept. of Agronomy, Tirana Albania; [2]University of Tirana, Dept. of Chmst. Albania; [3]FLOGEN Technologies Inc., 5757 Decelles Ave., Ste. 511, Montreal, QC H3S 2C3 Canada

Phytoremediation is a new low cost alternative technique for remediation of contaminated soils from heavy metals that are emitted by ferrous and nonferrous mining and extracting processes. It is based on the possibility to use several plants that accumulate high level of metals in order to remove metallic pollutants from soils and render them harmless. Phytoextraction is an adjacent new technique that uses these hyper-accumulator plants in order to extract the metals from them using even the conventional smelting or refining processes. In our previous work, an extensive investigation of about 150 plants have been carried and several species were identified that could be used for nickel phytoremediation and phytoextraction because of their high accumulation of nickel. It has been found that five taxa from Alyssum genus specie had the highest ability to accumulate nickel with concentrations more than 10000 µg/g (dry weight) or 1%. The taxa showing the highest accumulation of this metal is Alyssum murale var. chlorocarpum with 28 600 µg/g or 2.86%, a good candidate for Phytoextraction. In this work, in order to optimize the phytoremediation and phytoextraction processes further Absorption Spectrometry measurements and biological studies were carried out to determine the parts of the plants that accumulate the highest amount of nickel and the best biological cycle during which they accumulate the highest amount. The results show that the greatest accumulation of nickel occurred in the leaf material (2.86%) and the least in the roots (0.43%). The research on the biological cycle of the genus Alyssum showed that: (1) the seeds germinated between 5ºC to 30ºC and more in 25ºC; (2) 62.9% of seeds germinated at A.m. var. chlorocarpum; (3) the emergence is almost continue March to April; (4) the anthesis occurs from the May to July; (5) the ripening of the fruit take place 30 days after flowering; (6) the dissemination of fruit occurs from September to October. Due to these special characteristics it is reaffirmed that Alyssum murale var. chlorocarpum, as a nickel hyperaccumulator, is the most promising plant to be used for feasible phytoremedation and phytoextraction purposes.

Process Control and Optimization in Ferrous and Non Ferrous Industry: Feeds, Furnaces and Slags

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Monday PM — Room: Regency Ballroom D
November 10, 2003 — Location: Hyatt Regency Downtown Hotel

Session Chair: TBA

2:00 PM Invited

New Approach for the Optimization of Copper Concentrates Flash Combustion Through the Control of Blends and Slag Composition: *Roberto Parra*[1]; Florian Kongoli[2]; Roberto Parada[3]; [1]University of Concepción, Dept. of Metallurgl. Engrg., Edmundo Larenas 270, Concepción Chile; [2]FLOGEN Technologies Inc., Matls. Tech. Dept., 5757 Decelles, St.e 511, Montreal, QC H3S 2C3 Canada; [3]Compañía Minera Disputada, Chagres Smelter, Pedro de Valdivia 291, Santiago Chile

The operational control in a Flash Smelting Furnace is based on the mass and energy balance of the chemical and mineralogical composition of the concentrates. It is well known that many troubles in the dust formation and slag quality occur without a clear correlation to a specific process parameter such as the matte grade or heat balance. This paper outlines two new considerations that could both help improve the entire quality of the process: blend characterization and versatile slag composition control. Related to the blend control, laboratory scale study has shown that the magnetite and dust formation don't have a linear behavior with the weight proportion of the blend and some optimal blends of 2 or 3 types of concentrates can be identified. Related to the control of slag composition, the quantification of the slag liquidus temperatures and viscosity could be an effective operational tool for both for ferrite and fayalite slag that can also directly help deciding the blending parameters. From these viewpoints the benefits of the combination of these two approaches for high temperature operation is discussed.

2:25 PM

Modelling and Control of the Feed Preparation System of a Copper Flash Smelter: *Mikko Korpi*[1]; Hannu Toivonen[2]; Björn Saxen[1]; [1]Outokumpu Research Oy, Pyrometall., PO Box 60, FIN-28101, Pori Finland; [2]Åbo Akademi, Proc. Control Lab., Dept. of Chem. Engrg., Biskopsgatan 8, FIN-20500, Åbo Finland

The objective of this work was to identify a dynamic model for the feed preparation process behaviour. A sampling campaign was arranged to provide data for identification. The first approach is a fully stochastic adaptive prediction based on linear difference equations. The second approach is a deterministic blending tanks model where the dry concentrate silos and steam dryers are modelled as blending tanks. Further, a stochastic feature is added to the model and a Kalman filter is applied to estimate the compositions in the silos. The various models are validated using their ability to predict the feed mixture composition one hour ahead in time. Until now two online applications of these models have been produced on the smelter. The slag concentrate mass fraction is simulated with the blending tanks model and the composition of the feed mixture is estimated with the Kalman filter algorithm based on the blending tanks model.

2:50 PM Cancelled

Optimization of Coke Rate and Sintering Quality by Genetic Algorithm for Two-Layer Sintering of Iron Ore: *Niloy K. Nath*[1]; Kishalay Mitra[2]; [1]Tata Research Development and Design Centre, 54B Hadapsar Industl. Estate, Pune India; [2]Tata Consultancy Services, Mfg. Practice, 54B Hadapsar Industl. Estate, Pune India

3:15 PM Break

3:25 PM Invited

Examining Reheating Furnace Thermal Response to Mill Delays: *P. V. Barr*[1]; [1]University of British Columbia, Dept. of Metals & Matls. Engrg. Canada

Despite the advent of modern firing control systems reheating furnace operations still frequently allow significant thermal excursions in the discharged slabs or billets after furnace delays. Although HSM furnaces are not immune to this and other related problems, mini-mill operations are most vulnerable due to their more frequent delays and (often) less sophisticated control systems. In order to reduce these problems control systems will commonly include a thermal model, operating either on-line (interacting directly with the controller logic) or in an advisory off-line mode. Using a new 'fast' thermal model, the paper examines the thermal response of a typical mini-mill furnace during both delays and the subsequent recovery period. A variety of firing strategies are explored and compared on the basis of maintaining thermal excursions within allowable limits for rolling. Other factors, such as the potential for overheating of billets within the furnace during delays and the overall thermal state of the furnace, are also considered in some detail. Although common practice, the use of conventional thermocouple zone temperatures for furnace control during and after delays is shown to be a dubious proposition.

3:50 PM

Comparison of Different Control Strategies for Reheating Furnaces: *Chetan Premkumar Malhotra*[1]; [1]Tata Research Development & Design Centre, Proc. Engrg., 54/B, Hadapsar Industl. Estate, Pune, Maharashtra 411013 India

This paper describes an online control system and simulation environment for reheating furnaces. The simulator can be configured for implementing control using look-up tables, ideal heating curves and online look-ahead simulations. It is also used for offline generation of optimized normal operation and delay setpoints for look-up tables and generating ideal heating curves. Finally, it is employed to compare the performance of the three control strategies over a typical period of operation of a pusher-type reheating furnace.

4:15 PM Invited

Laser Off-Gas Measurement of CO, O2 and Temperature in EAFs: *Andreas Dietrich*[1]; [1]Linde AG, Linde Gas Div., SDM, Prod. Mgr. Mini Mills, Unterschleißheim 85716

The off-gas in the Electric Arc Furnace is measured online. A visualization screen shows the values of CO and Oxygen and temperature for the entire heat including the status of furnace equipment. The historical data for the heat are stored such that the furnace performance can be evaluated and optimized. A short comparison between laser based and conventional systems on the speed, influence of dust, water, pressure and the protection for bag house explosions is carried out. A high water and/or dust content in the sample does not present a problem with this type of system. The measurement works without interruption even under worst conditions (dirty scrap, carbon injection,...). The installation was developed in conjunction with Marienhuette, Graz. They are 100% scrap based with a tap to tap time of ca. 48 min.

4:40 PM Invited

Vaporization Processes and Thermodynamic Properties of Multicomponent Oxide Slags: *V. L. Stolyarova*[1]; [1]Institute of Silicate Chemistry of the Russian Academy of Sciences, ul. Odoevskogo 24, korp. 2, St. Petersburg 199155 Russia

The subject of the present study is multicomponent oxide slags that have the practical application in various fields of high temperature materials chemistry such as glass technology, metallurgy and incorporating of nuclear waste. Results of the investigations of the vaporization processes and thermodynamic properties of multicomponent oxide slags, containing SiO_2, B_2O_3, Al_2O_3, P_2O_5 and oxides of alkaline and rare-earth metals, that were obtained by the high temperature mass spectrometric method, allowed to make the following main conclusions concerning the composition of vapour over them at the isothermal conditions. 1. The systems formed by silica vaporize mainly as the individual oxides, for example as in the CuO-Na2O-SiO2 and CaO-TiO2-SiO2 systems. 2. Existence in the melts of boron oxide, P_2O_5, As_4O_6, Sb_2O_3 and oxides of alkali, alkali-earth metals, lead and bismuth at the concentrations of glass-forming oxide higher than the total concentration of oxide-modifiers leads to the appearance of gaseous salts of those elements. 3. In vapour over alkaliborosilicate systems at the concentrations of $M_2O> B_2O_3> SiO_2$ one can observe as the atoms of alkali metals and molecules ÌÂÎ2 è (ÌÂÎ2)2. The similar character of vaporization maintains in the four-component borosilicate systems, containing two alkali oxides, which can form the molecules of the mixed borates. Advantages of the application of the generalized lattice theory of associated solution and the approach based on the associated solutions model as the special case of it for the prediction of thermodynamic properties of multicomponent oxide systems were illustrated.

5:05 PM

Mathematical Model of Trace Contaminants Distribution in Copper-Nickel Production: *P. S. Seryogin*[1]; O. V. Korotkova[1]; L. Sh. Tsemekhman[1]; D. V. Rumyantsev[1]; [1]Kola MMC JS, Gipronickel Inst. JS Russia

For the purpose of increase in cost effectiveness a significant amount of secondary materials can be employed for processing of copper-nickel raw materials and semi-products. They may be the vehicle for such contaminants as zinc, lead, arsenic, tin and antimony entering into the technological circuit, and their content in ore feed is considerably lower than that in secondary raw materials. A presence of these impurities downgrades the quality of the end product. The contaminants distribution in the products of all the stages of Kola MMC production technology - ore-thermal smelting, copper-nickel mattes converting, high-grade matte flotation separation, oxidizing roasting in fluidized-bed furnaces, partial reduction in tube furnaces, anode electrosmelting, nickel concentrate reverberatory smelting, copper mattes converting, anode smelting, electrolytic refining of copper and nickel, slurries processing and sulphuric acid production - has been investigated under both laboratory and industrial conditions. On the basis of the specified distribution a mathematical model has been developed which allows to predict trace contaminants behavior in metallurgical production including dust processing, reverts, imported and a plant's own semi-products. With the use of such a model it is possible to predict the contaminants distribution in the products at any entry point of the impurities into the technological circuit. Usually the contaminants leave the process with waste products, most of all with ore-thermal smelting slag. The contaminants maximum permissible concentrations in the reverts depending on the amount of the contaminants entered into the production stage can be calculated with an aid of the developed mathematical model.

5:30 PM

Theoretical and Practical Aspects of the Direct Recycling of Slags in EAF Furnaces: *Petre Stelian Nita*[1]; [1]University "Dunarea de Jos" Galati, Faculty of Metall. & Matls. Sci., Romania

In small steelmaking shops, foundries and forging plants, there are not too many options for recycling of the basic slags since they have low chemical and structural stability which are not suitable for any recycling. An adequate recycling alternative is direct recycling in EAF. In this process, several quality requirements, physico-chemical properties and proportions of slags have to be analyzed. The progress in this field permits to establish an adequate proportion of recycled slag based on exact computation of the related property. For oxydizing slag, obtained during melting and in the first part of decarburization operation, the problem of phosphorus contents can be analyzed using the phosphate capacity ( ). For reducing periods, during deoxidization operation, desulphurization also occurs and the problem of the sulphur contents can be analyzed using the sulphur and sulphide capacities ( ). Between these two complex thermodynamic indicators of the slags, a direct relation is established by using thermodynamic aspects resulting from the equilibrium constants for dephosphorization and desulphurization process and also, by using the optical basicity of the slags that can be computed from the chemical analysis. On this basis, starting from the steels quality requirements, adequate strategies, measures and decisions can be established in order to control and optimize the process in order to obtain high rates of slag recycling such as 50-80% in direct steelmaking processes. Important cost savings can be obtained through this procedure based on the corresponding replacement of the fresh lime, iron ore and fluidizers amounts.

5:55 PM

Optimization of the Reverb Furnace Slag Composition in the RTB BOR Serbia: *Natasa Mitevska*[1]; Zivan D. Zivkovic[2]; [1]RTB BOR, Copper Inst., Zeleni bulevar 35, Bor 19210 Serbia; [2]University of Belgrade, Techl. Faculty, VJ 12, Bor 19210 Serbia

Copper lost in the reverberatory furnace slag is ireversible loss which increases with the copper content in the slag and the amount of the slag. Because of that it is necessary to optimize the discard slag composition which depends on concrete smelting conditions. It is very hard to select optimal slag composition. Even for the same type of raw-material, the optimal slag composition is not constant, for it depends on process parameters. Accordingly, for the optimal slag composition selection the characteristics of raw-materials, technological parameters, as well as all other, not less important, factors should be taken into consideration. The graphical optimization method is used and the optimal slag composition of the reverberatory furnaces No.1 and No. 2 in the RTB BOR, Copper Smelter and Refinery is obtained: (SiO_2) 38.0%; (FeO) 40.0%; (Fe_3O_4) 5.0%; (CaO) 5.0%; (Al_2O_3) 6.0%. It should be noted that this method has a lot shortcomings because it does not take into account other parameters which influence on the copper behavior during smelting process (physico-chemical characteristics of melts, technological parameters, distribution coefficient of copper, etc.)

Process Control and Optimization in Ferrous and Non Ferrous Industry: Molten Mattes, Metals and Aqueous Processing

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Tuesday AM — Room: Regency Ballroom D
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Session Chair: TBA

8:00 AM Invited

Optical Spectroscopy for Process Monitoring and Production Control in Ferrous and Non-Ferrous Industry: *Willy Persson*[1]; Wilhelm Wendt[1]; [1]Semtech Metallurgy AB, Ideon, Lund S-223 70 Sweden

A common feature of most pyrometallurgical processes is the injection of oxygen to remove various kinds and amounts of impurities present in the feed. The degree of success of a specific process step relies critically on control of the instantaneous oxygen potential/oxidation stage, throughout the step as well as upon termination of the step. This will, for instance, determine the distribution of impurities between metal and slag. As long as the operation is perturbation free detailed analysis of all additions and application of advanced models often yield satisfactory control means. However, a pyrometallurgical process is seldomly free from disturbances, which reduces the accuracy of the static models and leads to inconsistencies in the operation and variations in the output. Typical disturbances that might cause the process to leave the scheduled route might be uncontrollable changes in quality and quantity of feed, operator interventions and shift changes, timing of cranes, lining wear and accretions etc. The implementation of dynamic control to correct for disturbances and, more generally, for process optimization, requires continuous on-line information on the actual status of the process. The implementation of sensors for continuous process monitoring, e.g., as regards the instantaneously prevailing oxygen potential or oxidation stage, has been hampered by the highly aggressive environment in smelters. This is where remote-sensing techniques, based on optics and spectroscopy, has proven to form invaluable tools towards the realization of dynamic production control. Since about 15 years Semtech has developed and industrialized a remote-sensing technology, based on optics and spectroscopy, for continuous on-line process monitoring and production control of various pyrometallurgical processes. The presentation will discuss applicability aspects with examples and experiences from installations and tests in ferrous and non-ferrous industry.

8:20 AM

Ultrasonic Inclusion Detection and Cleanliness Measurement in Molten Aluminum and Magnesium: *Yuu Ono*[1]; Jean-Francois Moisan[1]; Yuanbei Zhang[2]; Cheng-Kuei Jen[1]; Chun-Yi Su[2]; [1]National Research Council of Canada, Industl. Matls. Inst., 75 de Mortagne Blvd., Boucherville, Quebec J4B 6Y4 Canada; [2]Concordia University, Dept. of Mechl. & Industl. Engrg., 1455 de Maisonneuve Blvd. W, Montreal, Quebec H3G 1M8 Canada

In lightweight metal processing such as aluminum (Al) and magnesium (Mg), metal cleanliness is a crucial process parameter for refining, part manufacturing and recycling in order to obtain high quality parts and products. In this paper, techniques for cleanliness evaluation of molten metals using ultrasonic probes with clad steel buffer rods having high signal-to-noise ratio (SNR) are presented. Due to the high SNR of the ultrasonic probes used, backscattered ultrasonic signals from inclusions, which may be oxide films and/or particles, in molten Mg and those from silicon carbide particles, having an average diameter of 50 microns, added in molten Al are successfully detected with reflection configurations of pulse-echo and/or pitch-catch modes at an ultrasonic frequency of 10 MHz. The movements of inclusions in the melts are also observed. In addition, relative cleanliness evaluation of molten Al and Mg is demonstrated.

8:40 AM

Accurate, Responsive Melt Rate Control During Vacuum Arc Remelting: *Rodney L. Williamson*[1]; Joseph J. Beaman[2]; David K. Melgaard[1]; [1]Sandia National Laboratories, 1835, MS 1134, PO Box 5800, Albuquerque, NM 87185-1134 USA; [2]University of Texas, Mechl. Engrg., Austin, TX 78712 USA

Vacuum arc remelting (VAR) is an industrial metallurgical process widely used throughout the specialty metals industry to cast large alloy ingots. Part of the VAR control problem consists of adjusting arc current to control electrode melt rate, which also depends on the electrode temperature distribution. Because the temperature distribution responds very slowly (2-4 hours) to changes in melt power, the melt rate response is history dependent and highly nonlinear. The situation is complicated further because measurement of the electrode temperature distribution is not practical. To solve the problem of accurate, responsive melt rate control, a low order, electrode melting model has been developed and incorporated into a VAR process controller. Data from laboratory and industrial tests show that the goal of responsive, accurate melt rate control has been achieved, even when melting under highly dynamic process conditions. The controller is able to maintain melt rate through electrode crack events.

9:00 AM

Solidification of Melt on a Rapidly Rotating Disc in Centrifugal Atomisation: *K. H. Ho*[1]; Y. Y. Zhao[1]; [1]University of Liverpool, Dept. of Engrg., Liverpool L69 3GH UK

This paper describes a simplified numerical model which is used to study the skull formation of liquid metal on a rapidly rotating disc in centrifugal atomisation. The skull formation is one of the problems limiting the wide use of centrifugal atomisation. The enlarging skull on the atomising disc reduces the yield of metal powder produced and produces a resistance to the centrifugal force which worsens the quality of the powder. It is costly and often difficult to study the flow behaviour by experiments due to the complex heat transfer and phase transformation during the processing. Computer modelling is therefore a powerful tool for mechanistic understanding of centrifugal atomisation. This paper investigates the flow pattern of the melt on the rotating disc as a function of initial temperature, melt flow rate and disc rotation speed as well as the physical properties of the melt, such as density, surface tension and viscosity using the commercial package Flow-3D.

9:20 AM Cancelled

Ladle Sculling Process Study on the Base of a Mathematical Model: *I. Yu. Petrovich*[1]; V. A. Blinov[1]; O. I. Zheldybin[1]; L. Sh. Tsemekhman[1]; Yu. A. Chumakov[1]; [1]Kola MMC JS, Gipronickel Inst. JS Russia

9:20 AM Invited

Role of CFD as a Process Monitoring and Prediction Tool for Secondary Steelmaking: *A. Mukhopadhyay*[1]; [1]FLUENT Inc., Centerra Resource Park, 10 Cavendish Ct., Lebanon, NH USA 03766-1442

Gas stirring, simultaneous arcing, chemical additions are some basic steps in the secondary steel making. From tap to team however, there are enough uncertainties and several in-situ decision making required to match the final composition an temperature in the given amount of processing time. Currently available control algorithms rely on overall material and heat balance coupled with a self-learning regression based tuning of model constants. In this paper we demonstrate the capabilities of Computational Fluid Dynamics (CFD) in modeling and analyzing the thermo-chemical aspects of secondary Steelmaking. These models take advantage of scientific and engineering advances in computational tools and provide almost real time speed of analysis. This can be a very effective tool for operator training, process debugging and improvement as well as new innovations.

9:40 AM Cancelled

Mathematical Model for Control of Autogenous Smelting of Copper Concentrate after High-Grade Matte Separation: *V. D. Zhidovetskiy*[1]; V. A. Blinov[1]; O. I. Zheldybin[1]; L. Sh. Tsemekhman[1]; L. B. Tsymbulov[1]; A. N. Golov[1]; [1]Kola MMC JS, Gipronickel Inst. JS Russia

9:40 AM

Column Flotation Scale-Up after Considering the Bubble Surface Area Flux: *R. Escudero*[1]; F. J. Tavera[1]; [1]Universidad Michoacana de San Nicolás de Hidalgo, Inst. de Investigaciones Metalúrgicas, Santiago Tapia 403, Morelia 48000, Michoacán México

The classical methodology to scale-up flotation columns by Finch and Dobby suggests the flotation rate constant (k) obtained through laboratory measurements remains during the design of a pilot or industrial unit. It has been presented in the literature a linear relationship between k and some dispersion characteristics such as gas holdup and the superficial bubble area flux (Sb). This work compares the recovery and grade results from experiments in a laboratory and pilot columns in the scaling-up by applying the traditional methodology with a new proposal that includes a mathematical expression relating Sb and k.

10:00 AM Break

10:15 AM Cancelled

Mathematical Model for Copper-Nickel Mattes Converting: *I. Yu. Petrovich*[1]; V. A. Blinov[1]; O. I. Zheldybin[1]; L. Sh. Tsemekhman[1]; Yu. A. Chumakov[1]; [1]Kola MMC JS, Gipronickel Inst. JS Russia

10:15 AM

Optimization of Downcomer Performance in the Jameson Cell by Measuring Electrical Conductivity: *F. J. Tavera*[1]; R. Escudero[1]; [1]Universidad Michoacana de San Nicolás de Hidalgo, Inst. de Investigaciones Metalúrgicas, Santiago Tapia 403, Morelia 48000, Michoacán México

Electrical conductivity in gas-water, and solids-gas-water systems was measured in the downcomer of a laboratory Jameson cell, to optimise the extension of the free jet zone, the mixing zone, and the plug flow zone, in terms of the gas hold-up characteristics, as a function of the gas and liquid (or slurries) flow rates. The effect of hydrophobic solids (coal) and hydrophilic solids (silica) was evaluated in the downcomer. Also, the effects of the downcomer performance on the phase distribution in the separation cell was evaluated by combining measurements of electrical conductivity and pressure to determine superficial velocities and hold-up.

10:35 AM

A Procedure for Chromate Conversion Coating of Commercial Galvanized Steel to Olive Color at Normal Temperature: *A. A. Mottahedi*[1]; [1]Iranian Aluminum Company (IRALCO), Kilometer 5 of Qom Rd., PO Box 31, Arak Iran

Chromate conversion coating is a process for making a complex layer at the surface of zinc galvanized steel which makes the metal more resistant to corrosion especially at marine atmosphere and increases the adhesiveness of color. In this work the influence of various compositions on commercial zinc galvanized steel sheet to the color of chromate conversion coating has been investigated at normal temperature and the factors that affect the control and optimization of the process have been determined. A bath composition of 20 g/liter Cr2O3 and 10 g/liter NaOH and a dipping time of 20 seconds at room temperature (25-30° C) make a desirable color of chromate coating. A slow agitation at a constant pH of 1 (with additions of NaOH or H2SO4) assures a constant bath condition and develops the color. This kind of coating has more corrosion resistance and this bath condition and compoisition are also more economical.

Process Control and Optimization in Ferrous and Non Ferrous Industry: Thermo-Mechanical Process Modeling: Deformation, Quenching, Casting and Welding

Sponsored by: Extraction & Processing Division, Materials Processing & Manufacturing Division, Jt. MPMD/EPD-Process Modeling Analysis & Control Committee, EPD-Pyrometallurgy Committee

Program Organizers: Florian Kongoli, FLOGEN Technologies, Inc., Materials Technology Department, Montreal, Quebec H3S 2CS Canada; Matthew John M. Krane, Purdue University, Department of Materials Engineering, West Lafayette, IN 47907 USA; Luis Ruiz-Aparicio, University of Pittsburgh, Pittsburgh, PA 15261 USA; Krich Sawamiphakdi, The Timken Company, R&D Manufacturing Technology, Canton, OH 44706 USA; Brian G. Thomas, University of Illinois, Department of Mechanical and Industrial Engineering, Urbana, IL 61801 USA

Tuesday PM Room: Regency Ballroom D
November 11, 2003 Location: Hyatt Regency Downtown Hotel

Session Chair: Krich Sawamiphakdi, The Timken Company, Canton, OH 44706 USA

2:00 PM Invited

Computer Modeling of Continuous Bar Rolling Mill: *K. Sawamiphakdi*[1]; P. M. Pauskar[1]; M. D. Conneely[1]; M. A. Soorma[1]; [1]The Timken Company, Timken Rsch., Canton, OH 44706 USA

A three dimensional finite element analysis program ROLPASM for modeling bar rolling has been enhanced for analyzing the continuous bar rolling process. The analysis is based on an Arbitary Eulerian Lagrangian method and a rigid-plastic material model. Based on the earlier work, the program includes the calculation of microstructure evolution providing accurate results of bar cross-sectional profile, rolling load, profile and history of temperature, strain, stress and austenitic grain size. A continuous bar rolling behavior is represented by applying front and back tension stresses at the front and back faces. A computer program to calculate front and back tension stresses from three consecutive rolling stands was developed. The calculated results were compared against physical measurements in the plant. Excellent agreement between the prediction and the measurements was obtained. The program is utilized to optimize new and existing roll pass designs.

2:25 PM

Mathematical Modeling of Formation of Cross-Sectional Wall Thickness Variations in Tubes During Their Cold Plug Drawing: Gennady I. Gulyayev[1]; Yu. G. Gulyayev[2]; Ye. I. Shifrin[1]; *K. Sawamiphakdi*[3]; [1]Osada State Tube Institute (DTI-VNITI), 1a Pisarzhevsky St., 5, Dniepropetrovsk 49600 Ukraine; [2]Nizhniednieprovsk Tubeworks, Dniepropetrovsk Ukraine; [3]The Timken Company, Canton, OH 44706 USA

Mathematical modeling of plastic deformation occuring in cold plug drawing of mother tubes with initial cross-sectional wall thickness variations (CSWTV) has been developed. The main provision of the model is that eccentricity [Em] is of such value that projection of all forces acting upon the plug in the deformation zone on axis OY perpendicular to the drawing axis OX equals zero. Calculations have proven that with other conditions being equal, increases in the die cone angle and deformation cycle number reduce CSWTV. Theoretical findings were confirmed by practical results.

2:45 PM

Visualizing the Evolutions of Microstructure Through Quenching Process: *Makiko Takahashi*[1]; *Mohammed Maniruzzaman*[1]; Richard D. Sisson[1]; [1]Worcester Polytechnic Institute, Matl. Sci. & Engrg., 100 Institute Rd., Worcester, MA 01609 USA

A tool is being developed to predict and visualize the microstructural evolution of steels during quenching. This tool utilizes experimental data and reference data that are stored in a database to predict the microstructural development. The visualization tool animates qualitative representation of two-dimensional microstructure drawings as well as the quantitative volume fractions of phases present as a function of time. This is achieved by superimposing the Jominy End-Quench test results over the Continuous Cooling Transformation diagram of the alloy. The predicted microstructure is presented through the web browser to maximize the ease of use. In addition, a parallel coordinate system is used to aid in identifying similarities within the data set by presenting the large number of data at a glance. The results for 4140 steel that was quenched in a wide variety of quenchants will be presented to illustrate the prediction and visualization tools.

3:05 PM Break

3:20 PM

Computer Simulation of Temperature and Thermal Stress Fields Generated During Heat Treating of JIS415H Steel Parts: *H. Castillo*[1]; M. A. Neri[1]; [1]Advanced Materials Research Center (CIMAV), Miguel de Cervantes N° 120, Complejo Industl. Chihuahua, C.P. 31109, Chihuahua México

This paper describes the computer simulation of thermal stress fields generated in the quenching of the JIS415H steel automotive parts (valve lifters), running the ANSYS multiphysics software of finite element (FEM). Simulations were performed introducing a residual stress measurements on specific valves areas, like internal pressure condition in the material. The stress condition effect in the material and the properties as temperature function data, were introduced to the FEM software. The thermal stress simulation was made on the 2D system. The parts were austenized to 850-900°C and then oil quenched, tempered at 150-200°C, and air cooled. The x-ray diffraction technique was made to take measurements from residual stresses on valves lifters surfaces. The results analysis showed the ideal stress condition, necessary in raw material, to reduce the scrap percent in grind operations after hardening heat treatment process.

3:40 PM

The Effect of Agitation on the Quenching Performance of a Quench Oil Using the CHTE Quench Probe System: *Mohammed Maniruzzaman*[1]; Mike Straton[1]; Thomas A. Rogers[1]; Lee P. Barber[1]; Richard D. Sisson[1]; [1]WPI, Matls. Sci. & Engrg., 100 Inst. Rd., Worcester, MA 01609 USA

The quenching performance of a liquid quenchant can be controlled by controlling the agitation in the quench tank. Without agitation, a vapor layer or bubbles form at the hot part surface and the natural convention of the quenchant limit the heat extraction rate at the quenched part surface. Resistance to the heat extraction rate can be reduced by breaking the vapor layer or by inducing a turbulent convection at the part surface through agitation (i.e. forced circulation of the quenchant). To determine the effects of agitation on the quench performance of a mineral oil based quenchant, the CHTE quench probe system was used with AISI4140 steel probe tip. Quenching performance of the oil is evaluated by computing the effective heat transfer coefficients of the steel probe as a function of surface temperature using Lumped Parameter Analysis. In addition, computational fluid dynamics (CFD) simulation of the quench tank with an impeller type agitator has been done to understand and predict the fluid flow pattern in the tank. CFD simulation also provides insights for determination of optimal location of the impeller and the quench probe tip. The experimental results have correlated with the CFD predictions in term of several dimensionless variables. These results are discussed in terms of theoretical model predictions of the effects of quenching fluid velocity on heat transfer between the steel part and the quenching fluid.

4:00 PM

Accurate Temperature Measurement During Water Quench Operations Characterized by Boiling Water Heat Transfer: *Dianfeng Li*[1]; Mary A. Wells[1]; [1]The University of British Columbia, Dept. of Metals & Matls. Engrg., 309-6350 Stores Rd., Vancouver, BC V6T 1Z4 Canada

A critical aspect of process control in industry is the development of representative mathematical models that can be used to optimize the operation in either an off-line or real time mode. Inherent to the accuracy of the model predictions is accurate knowledge of the boundary conditions in the process. In situations where water quenching is used to control the temperature of the product being produced, it is important to quantitatively understand the relationship between the heat transfer at the surface of the product during the quench operation. Typically this is done using a boiling water curve. Often these boiling curves are determined by using experimental measurements of temperature-time data in the product during a quench operation in conjunction with Inverse Heat Conduction (IHC) models. The experimental data used is often generated using thermocouples (T/C's) installed in the sample being cooled at either a sub-surface or surface location. This paper outlines different techniques for temperature measurement during quench operations and their associated impact on the local temperature field in the sample. The measurement techniques examined include both sub-surface as well as surface T/C's. Analysis of the errors associated with each temperature measurement method was done using both analytical solutions as well as a 2-D axisymmetric IHC model. The study showed that, during severe quench tests where the heat flux was very high, a surface T/C cannot be used as it acts as a cooling fin and produces a large error in the measured results. For measurements done using the sub-surface T/C's, the hole used to install the T/C must be taken into account in the analysis in order to obtain the accurate temperature-time data.

4:20 PM Invited

Process Control and Optimization of Near and Net-Shaped Aluminum-Silicon Alloys Premium Cast Products: *Reza Ghomashchi*[1]; [1]University of Quebec at Chicoutimi, CURAL, AMPRG, Dept. of Appl. Scis., Chicoutimi, Québec G7H-2B1 Canada

Casting is the most economical route to transfer raw materials into readily usable components. The economics of casting would be more pronounced and better realized, if there are no or limited necessary post fabrication treatments. Therefore, there is an urge towards near or net-shaped casting as there are significant advantages over conventional casting including reduction of component weight, excellent surface finish, higher strength and integrity of the as-cast parts, closer tolerance, and the ability to produce pore-free parts by controlling the solidification shrinkage. The concept of near or net-shaped casting is currently employed for both semi-finished products such as strip-casting and finished shaped casting, as in case of high pressure die casting or squeeze casting. The full potential of this process yet to be explored and is expected to be realized within the next 10 years, especially in case of strip casting. The current article discusses different near or net-shaped casting routes currently emp loyed for fabrication of high integrity finished products with main emphasis on aluminum-silicon alloys. In this regard, attempts will be made to identify the key parameters during fabrication and highlight the importance of process control and optimization in fabricating premium quality cast products.

4:40 PM

Multidisciplinary Coupled Simulations of Investment Casting Processes Using CASTS-FLUENT: *Juergen Jakumeit*[1]; Romuald Laqua[1]; Toni Ivas[1]; Joseph Scheele[1]; Markus Braun[2]; Aniruddha Mukhopadhyay[2]; [1]Access e.V., Intzestr. 5, Aachen 52072 Germany; [2]FLUENT, Hindenburgstr. 36, Darmstadt 64295 Germany

The coupled simulation of mold filling and solidification for an investment casting process is difficult due to the complexity of the different physical processes and the geometry. To handle this task in a precise way the CFD program FLUENT and the casting simulation tool CASTS were closely coupled. Any physical quantity like velocities or temperatures can be exchanged via files after each time step of the simulation. The communication and operating sequence of the programs is controlled by PERL-scripts. Hereby the expertise of FLUENT for flow simulation and the strength of CASTS for casting simulation could be combined. The coupled simulation was successfully applied to an aerospace investment casting. Several physical models were tested for a correct treatment of the casting filters, the porosity of the mold and the viscosity of the liquid metal. The results demonstrate that even complex investment casting geometries can be investigated using CASTS-FLUENT.

5:00 PM

Thermal Boundary Conditions for Computer Simulation of Grey Cast Iron Solidification in Sand Moulds: Niall Coone[1]; *David J. Browne*[1]; Martin Hussey[1]; Denis O'Mahoney[2]; [1]University College, Dept. of Mechl. Engrg., Belfield, Dublin 4 Ireland; [2]University College, Natl. Microelect. Rsch. Ctr., Cork Ireland

By exploiting the results of solidification modelling foundries can enhance the quality and reduce the cost of their casting processes. However not enough information exists on the thermal boundary conditions, which control the transfer of thermal energy stored in liquid metal to the mould via the metal/mould interface during solidification. This is quantified by the heat transfer coefficient (h.t.c.). An experimental and numerical study was carried out to find the magnitude and variation of the h.t.c. in cylindrical castings during the solidification of grey cast iron in green sand moulds. The h.t.c. values were calculated using a time marching solution to the inverse heat conduction problem. The variation of h.t.c. with metallostatic head was analysed. There is a wide scatter in green sand thermal properties due to the large number of variables involved in mould manufacture including green sand compaction and water content. The sensitivity of the calculation to uncertainties in the thermophysical properties of the green sand was evaluated.

5:20 PM

Casting Solidification and Coupled Thermo Mechanical Behaviour of a AlSi9Cu3 Investment Casting Alloy: *Eray Erzi*[1]; Suat Yilmaz[1]; [1]Istanbul University, Engrg. Faculty, Metallurgl. & Matls. Engrg. Dept., Avcilar Campus, Istanbul 34850 Turkey

Numerical analysis can efficiently and successfully solve complex and non-lineer problems like solidification of casting simulations. In this study, the investment casting of AlSi9Cu3 alloy were simulated by enthalpy model. By DSC (Differential Scanning Calorimetry) method the calorimetric properties and calculations of the temperature dependent enthalpy (latent heat) values of AlSi9Cu3 were experimentally measured especially at the liquid-solid phase change zone (mushy zone). Calculations consists of two steps. First, transient heat transfer analysis were made and solidification rates of casting that gained from the first step were also used as boundary conditions in the coupled structural analysis. As a result the thermo mechanical properties like the intensity and the directions of the stress and nodal displacements were reached by coupled structural analysis.

5:40 PM

Prediction of Evolutional Stress in Friction Stir Welding: *Changming Chen*[1]; [1]Southern Methodist University, Rsch. Ctr. for Advd. Mfg., Dept. of Mechl. Engrg., 1500 Internatl. Pkwy., Ste. #100, Richardson, TX 75081 USA

FSW is a relatively new welding process that may have significant advantages compared to fusion processes as follows: joining of conventionally non-fusion weldable alloys, reduced distortion and improved mechanical properties of weldable alloys joints due to the pure solid-state joining of metals, etc. In this paper, a three-dimensional model based on finite element analysis is used to study the evolutional stress in the butt-welding of aluminum alloy 6061-T6. The model incorporates the mechanical reaction of the tool and thermomechanical process of the welded material. The heat source involves the friction between the material and the probe and the shoulder. Thermal history and the evolution of longitudinal, lateral, and vertical stress in the friction stirred weld are simulated. The X-ray diffraction (XRD) technique is used to measure the residual stress of the welded plate, and the measured results are used to validate the efficiency of the proposed model. The relation between the calculated residual stresses of the weld and the process parameters such as tool traverse speed is presented. It is anticipated that the model can be extended to optimize the friction stir welding process in order to minimize the residual stress of the weld.

Process Control and Optimization in Ferrous and Non Ferrous Industry: Microstructure Modeling: Heating, Grain Growth and Precipitation

Sponsored by: Extraction & Processing Division, Materials Processing & Manufacturing Division, Jt. MPMD/EPD-Process Modeling Analysis & Control Committee, EPD-Pyrometallurgy Committee

Program Organizers: Florian Kongoli, FLOGEN Technologies, Inc., Materials Technology Department, Montreal, Quebec H3S 2CS Canada; Matthew John M. Krane, Purdue University, Department of Materials Engineering, West Lafayette, IN 47907 USA; Luis Ruiz-Aparicio, University of Pittsburgh, Pittsburgh, PA 15261 USA; Krich Sawamiphakdi, The Timken Company, R&D Manufacturing Technology, Canton, OH 44706 USA; Brian G. Thomas, University of Illinois, Department of Mechanical and Industrial Engineering, Urbana, IL 61801 USA

Wednesday AM　　Room: Regency Ballroom D
November 12, 2003　　Location: Hyatt Regency Downtown Hotel

Session Chair: TBA

8:00 AM Invited
Cementite and Carbide Dissolution in Steels During Austenitization at High Heating Rates: *T. C. Tszeng*[1]; G. Shi[1]; S. Purohit[1]; [1]Thermal Processing Technology Center, Dept. of Mechl., Matls. & Aeros., Illinois Inst. of Tech., Chicago, IL 60616 USA

Austenitization is a critical stage in heat treatment of steels. The available kinetic data in reference to various initial microstructures are very limited, particularly at high heating rates. In this study, integrated experimental and computational approaches have been conducted to quantify the progress of austenitization and the attained microstructure. In particular, the sudy is concentrated on cementite and carbide dissolution in two steel grades. Various computational methods are developed to facilitate the study: (1) an algorithm for direct determination of kinetics data as well as progress of transformation from high-rate dilatometer tests; and (2) a suite of mesoscale computational models for particle dissolution, elements diffusion, mechanics, thermodynamic and the resulting kinetics of transformation. Critical exprimentation is carried out using advanced techniques in microstructure characterization, chemical analysis, and Gleeble thermal-mechanical simulator on specimens of well-controlled initial microstructures.

8:25 AM
Process Design and Optimization for High-Temperature Carburizing: *X. Jay Gao*[1]; Gregory B. Olson[1]; Frode Stavehaug[2]; Christina Scharer[2]; [1]Northwestern University, Matls. Sci. & Engrg., 2220 Campus Dr., Evanston, IL 60208 USA; [2]QuesTek Innovations LLC, 1820 Ridge Ave., Evanston, IL 60201 USA

A fast high-temperature carburizing process integrated with materials design and optimization via a systems design approach was developed to significantly reduce process cycle time. Process experiments were focused on boost cycles to obtain a robust boost process and investigate surface reaction kinetics, primary carbide formation and dissolution. Weight gain and microhardness were measured, all showing evidence of non-monotonic time evolution for longer boost times at higher temperatures. Optical and electron microscopy and other techniques have been used to identify possible carbides, their location and types. These results assist the picking of first boost time with least variation rate in terms of content of case carbon and carbides, dissolvable in subsequent diffuse if any. The results also provide critical information to properly formulate surface reaction kinetics and diffusion and formation kinetics of carbides modeled using DICTRA.

8:50 AM
Grain Boundary Grooving by Surface Diffusion with Strong Surface Energy Anisotropy: T. Xin[1]; T. Xin[1]; T. Xin[1]; *Harris Wong*[1]; [1]Louisiana State University, Mechl. Engrg. Dept., Baton Rouge, LA 70803 USA

A vertical grain boundary intercepting a horizontal free surface forms a groove to reduce the combined surface energy of the system. We study grooving by surface diffusion with anisotropic surface energy. A recently developed delta-function model of facets is used to describe the surface energy with three or four fold symmetry. It is found that the groove grows following a similarity law. The self-similar groove profile is solved numerically by a shooting method. Even with strong anisotropy, the groove profile can be smooth if the exposed surface orientations do not include a facet orientation. The smooth self-similar groove shape is the same as an isotropic groove, but the size is reduced by a factor that depends on the degree of anisotropy. This induces a large error on the value of surface diffusivity if the isotropic model is used for an anisotropic system. In this talk, we will describe how to correct for this error.[1] [1]Xin, T. and H. Wong, "Grain-Boundary Grooving by Surface Diffusion with Strong Surface Energy Anisotropy," Acta Materialia 51, 2305-2317 (2003).

9:15 AM
Asynchronous Parallel Potts Model for Simulation of Grain Growth: *Priya A. Manohar*[1]; Anthony D. Rollett[1]; [1]Carnegie Mellon University, Matls. Sci. & Engrg., 4340 Wean Hall, 5000 Forbes Ave., Pittsburgh, PA 15213 USA

This work describes an implementation of the Potts model for simulation of grain growth in 2D and 3D on a distributed-memory parallel architecture. The simulation scheme utilizes continuous-time, asynchronous parallel version of the n-fold way algorithm. Each Processing Element (PE) carries a piece of the global simulation domain while the virtual topology of the PEs is in the form of a square grid in 2D and Torus in 3D. Different PEs have different local simulated times. Inter-processor communication is facilitated by the Message Passing Interface (MPI) routines. Sample results for grain growth simulation in 2D are presented for 720 x 720 global domain size distributed over 16 PEs. The grain growth kinetics obtained in the simulation of pure, isotropic systems demonstrates a close agreement with the analytical models. Grain size distribution obtained in the parallel simulation is well described by the expected lognormal distribution, thus validating the simulation procedure.

9:40 AM
Irregular Cellular Automata Modeling of Recrystallization and Grain Growth in an Al-Killed Steel Including the Influence of AlN-Precipitation: *Koenraad G.F. Janssens*[1]; Ernst Kozeschnik[2]; Fabiano Vanini[1]; [1]Swiss Federal Institute of Technology, Inst. of Virtual Mfg.,

ETH Zentrum CLA, Tannenstrasse 3, Zurich, Zurich CH-8092 Switzerland; [2]Graz University of Technology, Inst. for Matls. Sci., Welding & Forming, Kopernikusgasse 24, Graz A-8010 Austria

In the process of annealing a deformed metal the microstructure changes due to concurrent recrystallization, grain growth and precipitation. It is common knowledge that all three of these microstructural transformations show a strong dependence on each other, and that an overall model must take the relevant interactions into account. Aiming at the development of an approach which is useful in the more general case, a computational model is being developed which allows the prediction of the three dimensional grain topology and orientation distribution function of any metal submitted to subsequent deformation and annealing, taking into account concurrent recrystallization, grain growth and precipitation and starting from a statistical representation of the deformed microstructure. In this contribution a case study is presented which illustrates the potential and limits of the state of the art in the field.

10:05 AM Break

10:20 AM

Competing Processes of Hardening and Softening in Mild Steel: *Izendu Emenike Alu Aghachi*[1]; David H. Chandler[2]; [1]Technikon Pretoria, Dept. of Mechl. Engrg., PB X680, Pretoria, Gauteng Province 0001 S. Africa; [2]University of the Witwatersrand, Sch. of Mechl. Engrg., PB 3, Wits, Gauteng Province 2050 S. Africa

In static strain aging of low carbon steel, when the material is pre-strained, the dislocation density increases. If totally or partially unloaded and aged for a prescribed time, interstitial solute atoms diffuse under the influence of the dislocation stress fields, thus tending to lock the dislocations which causes an increase in yield stress. If held for long periods at a certain aging temperature, a decrease in yield stress (overaging) is observed following the initial increase. This behaviour has been variously attributed to either recovery of the cold worked dislocation structure and/or Ostward ripening of carbide precipitates. The present work demonstrates that, using a process control model for the competing processes of hardening and softening, dislocation recovery is responsible for overaging of mild steel specimens tested during the investigation.

10:45 AM

Modelling of Precipitation in Multi-Component, Multi-Particle, Multi-Phase Systems: *Ernst Kozeschnik*[1]; Jiri Svoboda[2]; Franz Dieter Fischer[3]; [1]Graz University of Technology, Inst. for Matls. Sci., Welding & Forming, Kopernikusgasse 24, Graz 8010 Austria; [2]Academy of Science of the Czech Republic, Inst. of Physics of Matls., Zizkova 22, Brno 616 62 Czech Republic; [3]Montanuniversitaet Leoben, Inst. of Mech., Franz-Josef-Str. 18, Leoben 8700 Austria

The simulation of the evolution of particles during heat treatment of industrial alloys has been a challenge to researchers for considerable time. Since such reactions can involve the concurrent nucleation, growth, coarsening and change in chemical composition of various types of precipitates at different positions in the surrounding microstructure, a treatment of these reactions becomes usually rather complex. Recently, a theoretical model has been developed that describes the evolution of such systems as a function of temperature and microstructure. The theoretical foundation of this novel model is based on Onsager's extremal thermodynamic principle which postulates that a thermodynamic system develops with a constraint maximum Gibbs free energy dissipation. Thus it is possible to simulate even complex precipitation sequences based on a numerical solution of the underlying rate equations. The theoretical model will be described briefly. Application of the model to ferrite formation at austenite grain boundaries as well as typical precipitation reactions in austenite will be presented.

11:10 AM

Simulation of Precipitation in a Complex 9-12% Cr Steel for Modern Steam Power Plants: *Joachim Rajek*[1]; Ernst Kozeschnik[1]; Horst Cerjak[1]; [1]Graz University of Technology, Inst. for Matls. Sci., Welding & Forming, Kopernikusgasse 24, Graz 8010 Austria

The novel multi-component, multi-particle, multi-phase precipitation model developed recently[1] is used to predict the precipitation kinetics in complex 9-12% Cr steels investigated within the European COST 522 project. These steels are used for tubes, pipes, casings and rotors in USC (ultra super critical) steam power plants for the 21st century. The calculation starts with a supersaturated austenitic matrix after the casting process. The simulation of the cooling process to the martensite start temperature including the nucleation, growth and coarsening of the typical precipitate populations like MX-particles, Cementite, M23C6 and other carbides is shown. After the austenite decomposition the matrix phase is switched into a ferritic/martensitic one and the following heat treatments are investigated in this second step. Finally, the evolution of the precipitate populations during long-term service at elevated temperatures are simulated where the main interest lies on the investigation of the concurrent growth and coarsening behaviour of different types of precipitates. The simulation results are compared to measured data obtained from the steel making process and long term creep tests. [1]ibid. E. Kozeschnik, J. Svoboda, F.D. Fischer, Modelling of precipitation in multi-component, multi-particle, multi-phase systems.

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Precipitation Kinetics of NbC in Ferrite of a Nb Microalloyed Steel: *Young-Kook Lee*[1]; [1]Yonsei University, Dept. of Metallurgl. Engrg., Shinchon-dong 134 Seodaemun-ku, Seoul 120-794 S. Korea

The precipitation kinetics of NbC in ferrite matrix of the Nb microalloyed steel was investigated experimentally and numerically. The mole fractions of NbC precipitates formed at different isothermal heat treatment conditions were measured by electrical resistivity test and were compared with both a mathematical model based on time-dependent nucleation and growth rates including interfacial energies between NbC and ferrite as a function of isothermal temperatures and the hardness. There is a good match among the calculated and measured precipitation kinetics of NbC and the hardness. The isothermal precipitation-temperature-time diagram of NbC in ferrite matrix of the Nb microalloyed steel was newly generated.

Process Control and Optimization in Ferrous and Non Ferrous Industry: Microstructure Modeling: Solid-State, Cooling Processes

Sponsored by: Extraction & Processing Division, Materials Processing & Manufacturing Division, Jt. MPMD/EPD-Process Modeling Analysis & Control Committee, EPD-Pyrometallurgy Committee

Program Organizers: Florian Kongoli, FLOGEN Technologies, Inc., Materials Technology Department, Montreal, Quebec H3S 2CS Canada; Matthew John M. Krane, Purdue University, Department of Materials Engineering, West Lafayette, IN 47907 USA; Luis Ruiz-Aparicio, University of Pittsburgh, Pittsburgh, PA 15261 USA; Krich Sawamiphakdi, The Timken Company, R&D Manufacturing Technology, Canton, OH 44706 USA; Brian G. Thomas, University of Illinois, Department of Mechanical and Industrial Engineering, Urbana, IL 61801 USA

Wednesday PM Room: Regency Ballroom D
November 12, 2003 Location: Hyatt Regency Downtown Hotel

Session Chair: TBA

2:00 PM

Prediction of Austenite Decomposition During Cooling of Low and Medium Carbon Low-Alloy Steels: *Ettore Anelli*[1]; Maria Cristina Cesile[1]; Paolo Emilio Di Nunzio[1]; [1]Centro Sviluppo Materiali S.p.A., Via di Castel Romano 100-102, Rome I-00128 Italy

Based on experimental CCT diagrams, an artificial neural network has been trained to predict the amount of microstructural constituents and hardness resulting from austenitizing and controlled cooling at rates from 150 to 0.01 K/s. It can be applied to quenching and normalizing processes of steels with 0.05-0.40 C% and 0.4-2.0% Mn with possible microalloying additions. Examples of the good predictive capabilities (standard deviation less than 15 Vickers for hardness and few volume percent for phases) are reported for tubular and long products.

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Computer Simulation of the Austenite-to-Ferrite Transformation in a Fe-20%Cr//Fe-7%Cr Diffusion Couple: *Anders Salwén*[1]; [1]Swedish Institute for Metals Research, Drottning Kristinas v. 48, Stockholm S-114 28 Sweden

In 1975 T. Nishizawa and A. Chiba reported on observed deviations from the ferrite-austenite local equilibrium in several diffusion couples based on the Fe-Cr system. In order to try to verify these results the austenite-to-ferrite transformation in a Fe-20 %Cr//Fe-7%Cr diffusion couple held at 1100 for 100 hours has been simulated. The simulation model is based on the postulated principle of maximum dissipation rate of Gibbs energy during transformation, which allows non-equilibrium interface conditions.

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Modeling the Formation of Bainitic Ferrite in Low-Carbon Steels: *Fateh Fazeli*[1]; Matthias Militzer[1]; [1]University of British Columbia, The Ctr. for Metallurgl. Proc. Engrg., 309-6350 Stores Rd., Vancouver, BC V6T1Z4 Canada

In low carbon TRIP steels, the formation of carbide-free bainitic ferrite is crucial for the stabilization of austenite. Based on experimental investigations and additional literature data modeling the bainite reaction is revisited for C-Mn-Si steels adopting both diffusional and displacive mechanisms. Transformation tests were carried out to study the isothermal austenite decomposition into bainitic ferrite for a model steel containing 0.6wt%C, 1.5wt%Mn and 1.5wt%Si which replicates the composition of remaining austenite at the start of the bainite reaction in a classical C-Mn-Si TRIP steel. In the diffusional approach, classical nucleation theory is employed and subsequent growth of bainite plates is modeled using the Zener-Hillert theory. The incorporation of the solute drag effect is discussed in terms of the modified Purdy-Brechet description. In the displacive approach, the autocatalytic nucleation of bainite plates is assumed to be rate controlling. The predictive capability of both models is evaluated for temperatures ranges where different morphologies of bainitic ferrite have been detected. The shortcomings and inherent challenges associated with either of these modeling approaches will be delineated.

3:15 PM Break

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3D FEM-Model for the Bainitic Transformation in TRIP-Aided Steels: *Danny Van Dooren*[1]; Philippe Thibaux[2]; Bruno Charles De Cooman[1]; [1]Ghent University, Lab. for Iron & Steelmaking, Technologiepark 903, Ghent 9052 Belgium; [2]OCAS NV, Arcelor Grp., John Kennedylaan 3, Zelzate 9060 Belgium

3D FEM modeling, which can predict the kinetics and micro-structural evolution during the bainitic transformation, has been developed. The input parameters are thermodynamic and atomic mobility data combined with structural mechanics data extracted from the stress-strain curves of the fcc and bcc phases present in TRIP steels. The model considers the bainitic transformation as a sequence of martensitic nucleation and growth of a ferritic subunit followed by carbon rejection into the surrounding parent austenite. The (re)-nucleation of the subunits is described through a non-classical martensitic nucleation criterion. The auto-catalytic effect of the presence of previously formed subunits is included into the nucleation criterion. Once a nucleus has been activated, a full-sized subunit is instantaneously formed through a displacive mechanism. The stress state is calculated by means of a 3D FEM programming code. After the formation of the subunit, 3D FEM programming was used to calculate the carbon diffusion from the supersaturated ferrite into the surrounding austenite. The resulting stress state and carbon profiles are inserted into the criterion for further nucleation.

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Strain-Induced Martensite Transformation in 0.2C-1.5Si-1.5Mn Steels - Influence of Strain Rate and Deformation Temperature: *A. Wasilkowska*[1]; D. Huckert[2]; E. Werner[1]; S. Traint[3]; A. Pichler[3]; [1]Technical University Munich, Christian-Doppler-Lab. for Modern Multiphase Steels Germany; [2]Grande École d'Ingénieurs, Inst. Natl. des Scis. Appliquées de Lyon, Lyon France; [3]voestalpine Stahl GmbH, Linz Austria

The microstructure of Si- and Al TRIP steels contains about 12 vol.% retained austenite with a mean grain size of 0.5 μm embedded in a fine-grained ferritic/bainitic matrix. Tensile tests were performed at different strain-rates and temperatures, and the mechanical properties and the fraction of retained austenite were evaluated. The investigated steels show a large total elongation (up to 40%) and an ultimate strength above 750 MPa, especially at low strain-rates and intermediate temperatures. The strain rate has a strong influence on the ductility, whereas its influence on the strength is moderate. The deformation temperature exerts opposite effects on the properties. The retained austenite to martensite transformation can be retarded at low strain rates and elevated temperatures. The high tensile strength and good ductility of TRIP steels make them candidate materials for automotive applications in light weight structural and high strength safety components.

4:20 PM

Theory, Validation and Application of a Microstructure Evolution Model Used for Hot Steel Rolling: *Richard A. Shulkosky*[1]; *David L. Rosburg*[1]; *Jerrid D. Chapman*[1]; [1]INTEG Process Group, Inc., 11279 Perry Hwy., Ste. 502, Wexford, PA 15090 USA

During the mid-90's, the American Iron and Steel Institute (AISI), in conjunction with the US Department of Energy (DOE) jointly funded the development of a microstructure evolution model for Hot Strip Mills. In 2000, INTEG Process Group, Inc. undertook the task of commercializing the technology. The Hot Strip Mill Model (HSMM) allows the user to easily set-up their mill configuration, including reheat furnaces, roughing mill stands, heat retention equipment, finishing mill stands, run out table and mill exit area. The model can be configured for reversing, continuous, tandem or Steckel mills. The model has a flexible system for handling a variety of steel grades. The HSMM uses a series of physical models to calculate both thermal mechanical and microstructure evolution. The enhanced HSMM was validated using a multitude of samples. Excellent agreement was obtained for yield strength, tensile strength and final ferrite grain size.

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Process Simulation Development for Industrial Rolling Applications: *Dave Lambert*[1]; Peter R. Jepson[2]; Hannu Pihlainen[3]; [1]SFTC, 5038 Reed Rd., Columbus, OH 43220 USA; [2]H.C. Starck Inc, 45 Industrial Place, Newton, MA USA; [3]Outokumpu Poricopper OY, R&D, PO Box 60, Pori Finland

Process modeling for large deformation metal forming processes has been developed into a very successful tool in commercial applications during the last two decades. DEFORM™ is a well-known metal forming process simulation program used by many industrial and research institutions. Recent developments include the ability to model multiple deforming body behavior during multi-pass pack rolling and microstructure prediction during multi-pass shape rolling. This paper summarizes how DEFORM™ can be applied to a number of rolling processes and briefly describes preliminary work carried out using the ALE technique.

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Microstructure Prediction in Thermo-Mechanical Processing by Multi-Scale Simulation: *Qiang Yu*[1]; Sven K. Esche[1]; [1]Stevens Institute of Technology, Dept. of Mechl. Engrg., Castle Point on Hudson, Hoboken, NJ 07030 USA

This paper reports on a research project supported by NSF, which aims at developing a multi-scale methodology for systematic microstructure prediction in thermo-mechanical processing. This methodology is based on combining mesoscopic microstructure models with macroscopic process formulations and involves the following three main steps: (1) based on the given global processing conditions, the gross deformation pattern of the entire workpiece is modeled using a continuum-based algorithm (such as FEM), (2) the resulting parameters are then extracted from the continuum-based simulation, post-processed and passed on to the mesoscopic numerical module, and (3) the microstructural changes are finally modeled (for selected zones or the entire domain of the workpiece) at the mesoscopic scale. This approach is expected to overcome the disadvantages of current microstructure prediction practice employing empirical relationships between microstructural features and processing parameters. It would ultimately provide universal and accurate prediction capabilities.

5:35 PM Cancelled

A Numerical Model of Thermokinetics of Technology Processes with a Phase Change: *Frantisek Kavicka*[1]; Josef Štìtina[1]; Bohumil Sekanina[1]; Pavel Ramik[1]; [1]Brno University of Technology, Faculty of Mechl. Engrg., Technicka St. 2, Brno 616 69 Czech Republic

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Microstructure of a Lead-Free Solder Alloy Sn-57.5Bi-0.5Ag Prepared by Foundry and Mechanical Alloying Processes: *M. A. Neri*[1]; [1]Advanced Materials Research Center (CIMAV), Miguel de Cervantes N° 120, Complejo Industrial Chihuahua, C.P. 31109, Chihuahua, Chih. México

A lead-free solder alloy Sn-57.5Bi-0.5Ag has been developed by mechanical alloying and foundry processes, and has great potential as a lead-free solder system, to low temperature applications. The mechanical alloying powders show a microstructure different to the microstructure obtained by the foundry process for the same alloy. Its melting point of 142°C is slightly higher than that of eutectic tin-bismuth solder. Examination of the microstructure revealed that eutectic microstructure is refined by the mechanical alloying process Ag additions. The lamellar structure of tin-bismuth gradually disappeared with the process of mechanical alloying, while intermetallic compounds Ag3Sn phase was formed. The Cu-Sn intermetallic compound layer formed at solder-copper interface is the Cu6Sn5 phase.