SYMPOSIUM C

Microstructural Modeling for Industrial Metals Processing

November 29 – 30, 1999

Chairs

Armand J. Beaudoin
Dept of Mech & Ind Engr
Univ of Illinois at Urbana-Champaign
354 Mechanical Eng Bldg MC-244
Urbana, IL 61801
217-244-9094

Paul R. Dawson
Sibley School of
Mechanical & Aerospace Eng
Cornell Univ
Ithaca, NY 14853
607-255-3466

Warren J. Poole
Dept of Metals & Mtls Engr
Univ of British Columbia
Vancouver, BC V6T 1Z4 CANADA
604-822-3674

Hugh Shercliff
Dept of Engr
Cambridge Univ
Cambridge, CB2 1PZ
UNITED KINGDOM
44-1223-332627

A Proceedings will be published with Symposium A as Volume 578 of the Materials Research Society Symposium Proceedings Series.

* Invited paper

SESSION C1: CASTING AND SOLIDIFICATION
Chair: Hugh Shercliff
Monday Morning, November 29, 1999
Room 209 (H)

8:30 AM *C1.1
GROWTH OF COLUMNAR DENDRITIC GRAIN STRUCTURE WITH FLUID FLOW (EBSD AND 3D CAFE MODELING APPLIED TO CONTINUOUS CASTING). H. Takatani[1,2], Ch.-A. Gandin[1,3] and M. Rappaz[1]; [1]Ecole Polytechnique Federale de Lausanne, Laboratoire de Metallurgie Physique, SWITZERLAND; [2]Mitsubishi Heavy Industries, Ltd., Hiroshima Research & Development Centre, JAPAN; [3]Ecole des Mines de Nancy, Laboratoire de Science et Genie des Materiaux Metalliques, FRANCE.

Columnar dendritic grains formed during continuous casting of thin steel sheets have been characterized by Electron Back Scattered Diffraction (EBSD) technique. It is shown that the grains have a random crystallographic orientation at the surfaces of the sheet in contact with the mold walls. In the middle of the sheet, the grains which have survived the growth selection mechanisms exhibit a $< 100 >$ texture in which the average dendrite trunk direction is not exactly aligned with the thermal gradient (i.e., the normal to the surfaces of the sheet). It is tilted by about 15 degrees toward the casting direction. This deviation is explained in terms of the apparent fluid flow velocity that the columnar dendrites see during solidification. This explanation is supported by simulations of grain structure formation based on a three-dimensional Cellular Automaton (CA) - Finite Element (FE) (3D CAFE) model which has been modified in order to account for fluid flow effects. The modified CA algorithm includes a growth kinetics of the dendrites which is a function of both the undercooling and fluid flow direction. It is validated by comparing the predicted shape of an individual grain growing under given thermal and fluid flow conditions with an analytical solution. The 3D CAFE predictions of the columnar grain growth in the presence of fluid flow are in good agreement with the experimental EBSD results.

9:00 AM C1.2
AN EFFICIENT PHASE CHANGE/FRONT TRACKING METHOD FOR DIRECT MICROSTRUCTURE SIMULATION. Damir Juric, Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA.

The development of an improved front tracking method for phase change problems is described and results of direct simulations of a variety of two-dimensional solidification systems both with and without fluid convection are reported. The solid/liquid interface dynamics in the simple diffusion governed dendritic solidification problem are treated using an imbedded Lagrangian interface description. Arbitrarily complex topologies and interface anisotropies are thereby directly and easily handled. The dendritic features simulated are quantitatively compared to an exact integral solution. Fully resolved simulations are attained on relatively coarse meshes. The phase change/front tracking method is then generalized to multiphase/multicomponent situations where the mass, momentum, energy and solute transport solution is fully coupled to the interface dynamics involving anisotropic surface energy, latent heat, solute rejection, interphase mass transfer and jumps in material properties. This technique is used to investigate the coupling of fluid and solid motion during the solidification of alloy grains.

9:15 AM C1.3
MODELLING OF GRAIN REFINEMENT IN ALUMINIUM ALLOYS. A.L. Greer, A. Tronche, M. Vandyoussefi, Univ of Cambridge, Dept of Materials Science and Metallurgy, Cambridge, UNITED KINGDOM.

Grain refinement by particle inoculation is a vital part of industrial processing of aluminium alloys. The present work focuses on DC casting of commercial-purity Al, though the basic concepts can apply also to shape-casting of alloys with higher solute contents. The aim is to develop a model for quantitative prediction of grain size as a function of: alloy composition, cooling rate, amount of added refiner and nature of the refiner. One interest in so doing is that with present refiners and refining practice, the efficiencies achieved are at best about 1% (i.e., only 1% of added particles acts as a nucleation substrate for a grain). In general, the modelling of nucleation is difficult, because key parameters (to which the nucleation frequency is very sensitive), such as the solid-liquid interfacial energy and the contact angle for nucleation on a substrate, are known imperfectly or not at all. In the present work it is shown that under the conditions usual in industrial grain-refining, i.e. very low undercooling, the barrier to free growth of a grain is set by the Gibbs-Thomson shift of the solid-liquid equilibrium, and not by the nucleation event per se. The present model is an adaptation of a model developed by Maxwell and Hellawell; it notes that grain growth on a nucleant particle affects the rest of system thermally, so that melt recalescence is the limiting factor for refiner efficiency. The model depends on knowledge of the nucleant particle size distribution. A measured size distribution is used and it is found that the predictions of grain size agree well with experiment. This work points the way to more accurate and physically based treatments of nucleation in casting models. Preliminary results on microstructural modelling obtained with *calcoMOS* will be presented.

9:30 AM *C1.4
A MODEL FOR PREDICTING WELD METAL GRAIN REFINEMENT IN GROWTH RATE-TEMPERATURE GRADIENT SPACE. Ø. Grong, Department of Materials Technology and Electrochemistry, Norwegian University of Science and Technology, Trondheim, NORWAY; and C.E. Cross, Department of Metallurgical Engineering, Montana Tech of The University of Montana, Butte, MT.

A theoretical model has been developed for use in predicting welding parameters that will favor grain refinement in weld metal. This model makes use of knowledge relating grain nucleation behavior to both cooling rate and nucleating particle density, assuming a condition of site saturation. Undercooling is taken to be related to the square root of growth rate. When plotted in logarithmic growth rate versus temperature gradient space (i.e. log R vs log G), one singe line will represent one particular cooling rate (RG = constant). Some where along this particular cooling rate line is a point representing the growth rate, and hence undercooling, where equiaxed nucleation may occur at a particular particle density. A lower particle density will require a higher growth rate, and undercooling, to achieve grain refinement. Thus, a grid may be constructed of intersecting lines defining where grain refinement may occur; one set representing variable cooling rates and the other set representing variable particle densities. This model will be discussed in comparison with other existing models. The effect of welding parameters on growth rate and temperature gradient will also be included in the discussion of this model.

SESSION C2: DEFORMATION AND TEXTURE
Chair: Paul R. Dawson
Monday Morning, November 29, 1999
Room 209 (H)

10:30 AM *C2.1
MICROSTRUCTURAL CHARACTERIZATION AND MODELLING. Niels Hansen, Xiaoxy Huang and Grothe Winther, Materials Research Department, Risø National Laboratory, Roskilde, DENMARK.

The evolution of dislocation structures in polycrystal with increasing strain is described within a framework of grain subdivision by dislocation boundaries and high angle boundaries. The evolving microstructure is characterized with emphasis on Morphology, the crystallographic and macroscopic orientation of the dislocation boundaries, their spacing and the misorientation angle across the boundaries. Such characterizations have shown correlations between the crystallographic orientation of grains and the deformation microstructure evolution, i.e. corrolation between the slip pattern and the microstructure. This finding opens up for microstructural modelling in metals processing, for example: 1) Formation and evolution of dislocation boundaries during forming, 2) slip pattern prediction based on microstructural observations and 3) coupling of microstructure and texture evolution. This line of microstructural modelling can link processing conditions via microstructure and texture to the macroscopic properties of metals and alloys. This link will be demonstrated by examples covering a number of metals and process parameters.

11:00 AM C2.2
COORDINATED EXPERIMENT AND SIMULATION FOR NON-UNIFORM DEFORMATION IN HOT WORKING OF ALUMINUM ALLOYS. M.E. Bange, A.J. Beaudoin, M. Stout, S.R. Chen and S.R. MacEwen, University of Illinois, Urbana, IL.

Multiple mechanisms, i) thermally-activated hardening and recovery, and ii) diffusion controlled solute drag, govern the deformation kinetics for hot working of AA 5182. For 6061 deformed under similar thermomechanical conditions, the dominant mechanism is thermally-activated hardening & recovery. An experimental model is posed that, in terms of complexity, falls between a homogeneous laboratory test and an industrial process. We show that constitutive equations for plasticity, describing different regimes of dislocation kinetics, can be used in conjunction with the finite element method to predict the mechanical response in a non-uniform deformation.

11:15 AM *C2.3
A CHARACTERIZATION OF THE STRUCTURE, PROPERTIES AND PERFORMANCE OF THICK ALUMINUM PLATE.

M.P. Miller, T.J. Turner, E.J. Harley, Sibley School of Mechanical Engineering, Cornell University, Ithaca, NY.

Thick rolled 7050 aluminum plate was developed for use in large component applications such as airframe bulkheads. Using the plate, significant cost savings can be realized by employing high speed machining to fabricate single-piece structures that are traditionally produced by assembling numerous, smaller parts. Because of the plate thickness and the inherent heterogeneity of its thermomechanical processing conditions, through-thickness microstructural gradients arise. Characterizing these gradients and modeling their effects on the properties and performance of the plate material are challenges that face airframe designers. In addition to other factors, one must understand not only the rolling-induced anisotropy that is commonly observed in rolled plate, but also its spatial variation. In this talk, we present the results from experiments designed to better understand the internal structure, properties and performance characteristics of AA 7050 plate in several gauges. We discuss a quantification of the crystallographic texture gradient in 120 mm thick plate made by taking individual lattice orientation measurements using the electron backscatter pattern (EBSP) technique. In addition to the through-thickness variation of the orientation distribution of the grains, there is a significant variation in grain size. These factors complicate the choice of optimal number of lattice orientation measurements which must be employed to quantify the orientation distribution function (ODF) field. We also examined the elastic-plastic deformation behavior of flat tensile specimens taken from various rolling direction (RD) transverse direction (TD) planes from several gauges of plate (50 mm - 200 mm). The specimen thickness and orientation were varied. We saw very little thickness-dependence in the stable stress-strain curves. As expected, the thicker specimens deformed to larger strains, however. We saw significant anisotropy (strength and ductility) in these machined sheet specimens that varied with plate gauge and specimen location. The localization behavior and general post-test appearance of specimens with axes in TD were markedly different than those oriented in RD. Current studies are being conducted to explore the microstructural sources of these anisotropies.

11:45 AM C2.4
CRYSTALLOGRAPHIC TEXTURE AND YIELD BEHAVIOR OF Al-Cu-Li (2195) PLATE. Karen Crosby, Su-Seng Pang, Louisiana State Univ, Dept of Mechanical Engineering, Baton Rouge, LA; Reza Mirshams, Southern Univ, Dept of Mechanical Engineering, Baton Rouge, LA.

Existing experimental texture analysis capabilities allow testing of theories on plasticity using polycrystal models. Aluminum-lithium alloys, which are particularly suited for aerospace applications due to excellent strength to weight ratio, typically possess pronounced textures. Al-Cu-Li (2195) thick plates were deformed by cold rolling to various thickness reductions. The plates exhibit a texture gradient through the plate thickness accompanied by a variation in yield strength values. The difference in yield strength values is related to the texture variation in terms of the texture components (ideal crystallographic orientations) identified from experimental measurements. A modified Taylor-based polycrystal plasticity model developed by Kocks and his colleagues is used to predict yield surfaces by incorporating texture data. Results of this investigation show that the texture intensities measured at certain ideal orientations increase or decrease with increasing deformation. These textural changes influence the value and anisotropy of the yield strength of the alloy.

SESSION C3: DEFORMATION AND TEXTURE
(continued)
Chair: Armand J. Beaudoin
Monday Afternoon, November 29, 1999
Room 209 (H)

1:30 PM C3.1
ON THE INFLUENCE OF HETEROGENEOUS DEFORMATIONS ON TEXTURE EVOLUTION IN METAL POLYCRYSTALS. Paul Dawson, Nathan Barton, Sibley School of Mechanical and Aerospace Engineering, Cornell University, Ithaca, NY.

In metal deformations, heterogeneity in straining occurs over a variety of physical length scales. Here we focus on two, that of characteristic dimensions of a workpiece and that of dimensions typical of polycrystals that constitute representative samples of the material drawn from the workpiece. We discuss simulations of evolving microstructure using crystal plasticity and finite element methods to model rolling processes for titanium and titanium alloys (single and two phase systems). Titanium is a demanding material to model owing to the high level of single crystal anisotropy of the hexagonal close packed phase and to the large difference in strength between the hexagonal close packed and body centered cubic phases. At the level of a polycrystal, the influence of constraints imposed by neighboring crystals on the evolution of crystallographic texture is presented, both in terms of the overall texture and on features of the intercrystalline misorientations. At the level of the workpiece (rolled plate), we examine the influence of varying deformation path through the thickness of the plate on the strength of texture gradients. Comparisons to textures measured for rolled titanium are presented.

1:45 PM *C3.2
EVOLUTION OF GRAIN SIZE ON RECRYSTALLISATION DURING HOT ROLLING OF AUSTENITIC STAINLESS STEELS. J.A. Whiteman and C.M. Sellars, IMMPETUS (Institute for Microstructural and Mechanical Process Engineering: The University of Sheffield), Sheffield, UNITED KINGDOM.

During hot rolling of austenitic stainless steels complete static recrystallisation is expected between passes unless finishing temperatures are low. Typically progressive refinement from pass to pass takes place to grain sizes in the range of 20-50 μm. However, most experimental studies of the effects of strain, strain rate, temperature and initial grain size on recrystallisation kinetics and recrystallised grain size under hot working conditions have been carried out on initial grain sizes greater than 50 μm. Empirical relationships from these data and from more limited results of C-Mn steels have been extrapolated to smaller grain sizes for use in models of microstructural evolution during rolling.
Recent development of a physically based model for the effects of initial grain size, assuming that site saturated nucleation occurs on grain corners, grain edges, grain faces and at intragranular sites leads to interdependence of the effects of strain and grain size on nucleation density and hence on recrystallised grain size and recrystallisation rate. Experimental evidence available in the literature and some new results on finer grained Type 316 stainless steel are reviewed and compared with the expectations from the model.

2:15 PM *C3.3
THE CELLULAR AUTOMATON SIMULATION OF MICROSTRUCTURAL EVOLUTION DURING DEFORMATION PROCESSING OF METALS. Chris H.J. Davies, Department of Materials Engineering, Monash University, Clayton, VIC, AUSTRALIA.

The computer simulation of the evolution of microstructure during deformation processing is a desirable but elusive goal. In order to be effective, models must be tied to deformation parameters (temperature, strain rate, strain), and grain size distributions and recrystallisation kinetics must be predicted with high accuracy if the evolution of microstructure is to be tracked through several passes. This paper examines the cellular automaton (CA) simulation technique which has the potential to enable the modeller to accomplish these goals.
Aspects of the CA technique examined are the three dimensional representation of microstructure and its evolution, the incorporation of texture representation into simulations, and the development of simulations of precipitation events. Also investigated will be the limitations of the technique, in terms of the error that can be expected when different boundary conditions are imposed on a simulation. Although at a rudimentary stage of investigation, the interfacing of CA simulations with deformation simulations (eg, finite element) will be examined. The paper concludes with a discussion of the challenges facing the implementation of CA simulations in industrial process models.

3:15 PM C3.4
MODELING DISLOCATION CELL STRUCTURE EVOLUTION. Mark A. Miodownik, Elizabeth A. Holm, Sandia National Labs, NM; David J. Srolovitz, University of Michigan, Materials Dept, MI; Peter Smereka, University of Michigan, Math Dept, MI.

Plastic flow in metals occurs by a dislocation mechanism in which strain is accommodated by a dislocation flux. This results in tangled networks of dislocations which self-organize into stable cell structures. These structures have a number of remarkable properties not least of which is that they exhibit scaling. We examine the idea that the evolution of these dislocation cells is dominated by random fluctuations and that pattern formation arises from this complexity. We construct a simple model of the evolution of cell orientations and show that scaling of misorientation distributions is a direct result of random fluctuations. The results are compared with the experimental measurements and show excellent agreement. This novel approach to deformation substructure evolution occupies a niche between discrete dislocation simulations and FEM plasticity codes.

3:30 PM C3.5
THE LINKAGE BETWEEN MESOSCALE MATERIAL INHOMOGENEITY AND DEFORMATION-INDUCED SURFACE

TEXTURE IN SHEET METALS. Xianghong Li, Changjin Xie, Wei Tong, Yale University, Dept. of Mechanical Engineering, New Haven, CT.

It has been experimentally observed that surface plastic strain distribution becomes noticeably non-uniform at a length scale equal to or less than the thickness of a polycrystalline sheet metal. Such non-uniform plastic strain patterns are found to correlate reasonably well with the variation of surface topography of the sheet metal at the similar length scale. A sheet metal plasticity model is formulated with the inclusion of certain planar mesoscale material inhomogeneities that are larger than individual grains. A finite element analysis incorporating such a sheet metal model is carried out and the correlation between the surface plastic strain inhomogeneity and surface texture is established. Implication of mesoscale material inhomogeneities on surface finish and ductility of sheet metals is examined.

3:45 PM C3.6
PREDICTED EVOLUTION OF A FLOW SURFACE BY A POLYCRYSTAL PLASTICITY DEFORMATION MODEL. Thomas E. Buchheit, Materials Aging and Reliability Dept. and Gerald W. Wellman, Engineering and Manufacturing Mechanics Dept. Sandia National Laboratories, Albuquerque, NM.

A rate dependent material model which resolves plastic deformation to crystallographic slip systems of FCC metals has been implemented into JAS-3D, a quasistatic, large deformation, nonlinear finite element code developed at Sandia National Laboratories. The resultant microstructural based elastic-plastic deformation model has successfully performed simulations of realistic polycrystalline microstructures generated using a Potts model approach. Three dimensional polycrystalline simulations have been as large as 50,000 elements with several hundred elements per grain. Consequently, they provide detailed microstructural information during deformation simulations, such as local stress, strain and subgrain orientation distributions. In this study, simulations of polycrystals composed of 200 grains with approximately 200 elements per grain have been performed to determine the predicted evolution of the plastic flow surface during tensile deformation of OFE Copper. The flow surface evolution using isotropic and latent slip system hardening models was investigated. The isotropic hardening model allows each slip system to harden equally, however, grain neighbor interactions impart local subgrain orientation changes and material flow strength variations within grains, driving an anisotropic polycrystalline flow surface evolution. In contrast to the straightforward isotropic model development, the latent hardening model uses differential slip system hardening ratios derived from single crystal experiments, an effect which could significantly contribute to the anisotropic evolution of mechanical properties in a polycrystal. A comparison of flow surface evolution predictions using both models will be given with reference to available experimental data. The presentation will conclude with a discussion of using the analyses for developing phenomenological relationships in finite element simulations of large scale deformation processing operations. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

SESSION C4: POWDER AND SPECIAL PROCESSES
Chair: Warren J. Poole
Monday Afternoon, November 29, 1999
Room 209 (H)

4:00 PM C4.1
NUMERICAL SIMULATION OF MICROSTRUCTURAL EVOLUTION DURING SINTERING - I. MODEL. Veena Tikare, Michael Braginsky, Sandia National Laboratories, Albuquerque, NM; Eugene A. Olevsky, San Diego State University, San Diego, CA.

Sintering theory has been developed either as the application of complex diffusion mechanisms to a simple geometry or as complex evolution of microstructure with simple diffusion mechanisms. In this paper, we present a model that can treat in detail both the evolution of microstructure and the sintering mechanisms of a realistic powder compact. We have incorporated the stereological theory of sintering in a lattice-based, Monte Carlo model, also know as the Potts model. The stereological theory of sintering describes the evolution of individual stereological constructs such as the grain boundary and pore-grain interface given the mass transport mechanisms. However, it cannot track the changes at all such boundaries in a complex geometry. Incorporation of the stereological model into the Potts model allows us to track microstructural changes in a complex and realistic geometry. In this paper, we will review the stereological theory of sintering and its application to microstructural evolution. We will then demonstrate how these stereological concepts and diffusion mechanisms were incorporated into the Potts, Monte Carlo model to simulate sintering. We will present this modified Potts model which can simulate grain growth by bulk diffusion, pore coalescence by surface diffusion and densification by pore annihilation driven grain boundary diffusion. This work was performed at Sandia National Laboratories under the contract DE-AC04-94AL-85000 to U.S. DOE

4:15 PM C4.2
NUMERICAL SIMULATION OF MICROSTRUCTURAL EVOLUTION DURING SINTERING - II. APPLICATION & DEVELOPMENT OF CONSTITUTIVE CONTINUUM RELATIONS. Michael Braginsky, Veena Tikare, Sandia National Laboratories, Albuquerque, NM.

A modified Potts numerical algorithm incorporating stereological model of microstructural evolution is used to simulate sintering in a powder compact. We present results of numerical simulations, including sintering kinetics and densification. In addition, we discuss ways to construct, based on these simulations, constitutive equations for macroscopic continuum models. As an example, constitutive equations for a continuum model of sintering with microstructure characterized on the macroscopic level by the specific volume ($1/\rho$, where ρ is the volumetric mass of porous material) are determined on the basis of our numerical simulations. This work was performed at Sandia National Laboratories under the contract DE-AC04-94AL-85000 to U.S. DOE.

4:30 PM C4.3
THIXOTROPY OF SEMISOLID METALS. Andreas Alexandrou, Gilmer Burgos, SSMP Lab - Metal Processing Institute, WPI, Worcester, MA; Vladimir Entov, Institute for Problems in Mechanics of Russian Academy of Science, Moscow, RUSSIA.

Processing of metal alloys in their mushy state represent a new trend in metal processing. Low porosity, high crack resistance along with fine and homogeneous microstructure obtained by this process, results in components with mechanical properties better than those produced by casting and comparable to those of forged alloys. Understanding the time-dependent flow behavior of metal alloys in semisolid state is essential for the further development of the process. Semisolid slurries can be defined as highly concentrated suspensions of alpha phase in eutectic liquid of slightly different composition. At high solid fraction, the alpha phase forms a skeleton of interconnected solid particles, and the apparent mechanical behavior of the system is primarily determined by the structure and properties of the skeleton. The structure is almost never at equilibrium, it depends on the mechanical and thermal history of the material, and its evolution is governed by a number of kinetic phenomena of different characteristic time-scales. As a result of these kinetic processes, the rheological properties of the material, such as effective viscosity and yield stress, decrease with structure breakdown and increase with its development. In the present investigation, the thixotropic behavior of semisolid slurries is modeled using conservation equations and the Herschel-Bulkley fluid model. The rheological parameters are assumed to be functions of the solid volume fraction and a structural parameter that changes with the processing history. The evolution of the structural parameter is described by a first order kinetic differential equation that relates the rate of build-up and break-down of the alpha phase skeleton. The model is implemented into a finite element code to predict die filling. An extensive parametric study is performed and their effect on processing is analized. It is concluded that common problems encountered in filling processes of semisolid metals can be avoided by appropriate control of the rheological parameters.

4:45 PM C4.4
DEVELOPMENT AND VALIDATION OF A COMPUTATIONAL MODEL OF DROPLET IMPACT. Donna L. Hale, Ray A. Berry, Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID.

An adapted particle-in-cell method has been developed to simulate the high deformation during the impact of a molten droplet. Modeling the deposition dynamics of a single droplet is the first step towards understanding the evolution of a coating microstructure, since a coating is built up from the successive accumulation of many deformed, solidified droplets. Validation of the numerical method is accomplished using separate effects testing. Since the model simulates a non-linear, complex process, a series of much simpler test cases have been implemented to thoroughly test each feature of the code. The computational algorithm consists of an initialization phase, a Lagrangian phase, and a convective phase. Conservation of momentum and energy equations are solved in a Lagrangian reference frame, where computational particles representing a single droplet are overlaid on a fixed, Eulerian grid, and advection is accomplished by moving the particles. This technique avoids mesh distortion and the need to continuously remesh to capture the large deformations. The effects of compressibility were tested to simulate wave propagation

within the droplet at impact. The artificial viscosity method of Wilkins and the conservative smoothing technique of Lapidus were employed to damp numerical oscillations. Computed conduction heat transfer profiles are compared with an analytic solution. Release of latent heat upon solidification is incorporated into the energy equation using a temperature-energy map. The solidification interface evolves naturally from the energy equation and is not constrained to rise in a planar fashion from the substrate as in other models. In this paper, validation of the numerical predictions made by the code are described in detail.

SESSION C5: THERMAL PROCESSES AND PHASE TRANSFORMATIONS
Chair: Hugh Shercliff
Tuesday Morning, November 30, 1999
Room 205 (H)

8:30 AM *C5.1
CHARACTERIZATION AND MODELING OF PRECIPITATION KINETICS IN ALUMINUM 7000 ALLOYS. Alexis Deschamps, Jens C. Werenskiold, LTPCM / ENSEEG, Domaine Universitaire de Grenoble, St. Martin d'Heres, FRANCE.

The precipitation kinetics in the aluminum alloy 7108.70 used for automotive applications is investigated in a wide range of temperatures (100 to 170 degrees C) corresponding to the range of industrial processing. Experimental procedures include TEM for the nature and distribution of precipitates, and in-situ Small Angle Xray scattering for the quantitative determination of precipitate sizes and volume fractions. An internal-state variable model which predicts the evolution of microstructural parameters such as average radius and volume fraction of precipitates is applied to this series of data. The parameters of the model, which have a physical meaning, are discussed in relation with the physical phenomena occurring over this temperature range.

9:00 AM C5.2
A PROCESS MODEL TO PREDICT YIELD STRENGTH FOR 7030.60 AND 7108.72 ALUMINUM ALLOY USED IN AUTOMOTIVE BUMPER APPLICATIONS. W.J. Poole, J. Huang, University of British Columbia, Dept. of Metals and Materials Engineering; J. Saeter, Hydro-Aluminium Research Centre; S. Skjervold, G. Waterloo, Hydro-Raufoss Automotive Research Centre.

A process model has been developed to predict the yield strength of 7030.60 and 7108.72 aluminum alloy after fabrication and heat treatment. The fabrication of these alloys involves a stretch forming process immediately after solution heat treatment followed by natural ageing and then a two step artificial ageing heat treatment. Experiments have shown that there is a strong interaction between the precipitation hardening behaviour and the level of cold work introduced during fabrication. Some of the key observations from experiments are that the peak strength due to precipitation is lowered in the presence of cold work, the kinetics of precipitation are accelerated and that substantial recovery of the cold work occurs. An internal state variable model has been developed to predict the strength for a pre-strain in the strain range of 0-1.2 and artificial ageing treatments between 100-180°C (with emphasize on the two-step treatments). The lowering to the peak strength is attributed to a widening of the precipitate size distribution and the increased kinetics are accounted for by an enhanced diffusion rate due to the pipe diffusion from the increased dislocation density. The model uses the concept of kinetic strength to handle non-isothermal ageing treatments and also accounts for recovery of the cold worked structure in a preliminary manner. Very good agreement is observed between experiments and the predictions from the model.

9:15 AM C5.3
MODELING THE BEHAVIOR OF ALUMINUM ALLOY 319 DURING HEAT TREATMENT. Matt Newman, Jonathan A. Dantzig, Huseyin Sehitoglu, Dept. of Mechanical and Industrial Engineering, University of Illinois, Urbana-Champaign, IL.

Weight reduction has led to the replacement of steel by aluminum in many automotive applications. In this work, a low-cost aluminum alloy (319) is studied. The use of aluminum 319 in these conditions requires that parts undergo a precipitation heat treatment which involves a quench followed by aging. Parts subject to this heat treatment are prone to residual stresses and deformations due to the large thermal gradients imposed by the quench. It is desirable to model the behavior of the aluminum during heat treatment in order to predict these residual stresses and deformations. To accurately model this behavior, material properties must be correctly portrayed at different stages of the process. Both initial microstructure (secondary dendrite arm spacing) and evolving microstructure (precipitation and coarsening) should be taken into account. In the material model, a state variable based on microstructural changes associated with precipitation and coarsening is used to predict the increase in resistance to deformation with straining. Secondary dendrite arm spacing appears in the form of parameters derived from uniaxial tensile tests. The material model is incorporated into both semi-analytical and finite element codes in order to predict deformation of a quenched aluminum beam. Numerical results are compared with experiments.

10:00 AM *C5.4
MODELLING OF MICROSTRUCTURE EVOLUTION DURING HOT STRIP ROLLING. M. Militzer, I.V. Samarasekera, W.J. Poole, Univ of British Columbia, Dept of Metals and Materials Engineering, Vancouver, CANADA.

The microstructure evolution has been modeled for hot strip rolling of advanced low carbon steels with microalloying additions of Nb, Ti and/or V. The microstructural model has been combined with temperature and deformation models to predict the mechanical properties of hot rolled steel as a function of the operational parameters in a hot strip mill. To aid the model development, experimental studies were performed in the laboratory including hot torsion tests to simulate the entire hot rolling process from reheating to coiling and a variety of tests employing a Gleeble 1500 thermomechanical simulator to characterize the individual microstructure phenomena of recrystallization, grain growth, precipitation and phase transformation. The critical processing step for development of the final properties of hot rolled steels is cooling after rolling. In this step, the austenite-to-ferrite transformation and the precipitation of microalloying additions occur and these events determine the final microstructure. Thus, the microstructural model emphasizes the kinetics of transformation and precipitation. A fundamental nucleation and early growth model is proposed to predict the start of the ferrite formation. Ferrite growth rates can adequately be described by a carbon diffusion model taking into account a solute-drag-like effect of Mn and Nb. Alternatively, a semi-empirical approach can be used employing the Johnson-Mehl-Avrami-Kolmogorov model and adopting additivity. The ferrite grain size is essentially determined at the early stages of transformation and can, therefore, be expressed as a function of the transformation start temperature. Precipitation occurs in ferrite during slow cooling of a coil. Precipitation strengthening kinetics due to carbides and nitrides of Nb, Ti and V is controlled by particle coarsening. The ageing behaviour can then be described based on the Shercliff-Ashby model for precipitation hardening. The predicted microstructures and properties agree well with data obtained from industrially rolled coils.

10:30 AM *C5.5
DANTE: A THERMOMECHANICAL/KINETICS SIMULATOR OF THE HEAT TREATMENT OF LOW ALLOY STEELS.
Mark T. Lusk, Young-Kook Lee, Colorado School of Mines, Div. of Engineering, Golden, CO; Vince Prantil, Sandia National Laboratory, Livermore, CA.

Simulation of the heat treatment of low alloy carbon steels requires predictive models that couple thermomechanical processes with five distinct phase transitions and product phase tempering. The modeling strategy adopted here couples differential equations for phase evolution and tempering with a multiphase macroscopic state variable material model. The kinetic rate equations are derived using a thermodynamic formulation fit to experimental data. The kinetics model is validated using time temperature transformation and continuous cooling transformation data, and by studying the influence of stress on the kinetics through compression and tension experiments. The elastic-plastic constitutive behavior is highly nonlinear. In particular, at high temperatures, the material has very low yield strength and can readily flow plastically. During transformation, product phases such as martensite are substantially harder than the parent austenite. This drives further plastic straining in the austenite when under stress, a phenomenon referred to as transformation induced plasticity (TRIP). The yield and hardening behavior depend on the carbon content, temperature and strain rate. The transformation strains also depend upon carbon content and temperature. Finally, the lattice volume expansion upon carburization is of the same order as the transformation strains and contributes significantly to distortion. The mechanical model used in this research is based on a mixture theory, wherein we track the behavior of individual phases using a state variable formulation for elasto-plasticity. This model is coupled to a new differential approach to simulating phase transformation kinetics. Phase interactions are accounted for by introducing TRIP that accounts for both the macroscopic multiphase behavior and effects driven by the transformation.