

Fundamentals of High Temperature Processes**Molecular dynamics simulation of dilute solutions of MeO and MeF₂ in the CaO-CaF₂ system***D.K.BELASHCHENKO et al.*

Models of oxide-fluorides CaO-CaF₂ with additions of MeO and MeF₂ were constructed and investigated by molecular dynamics method at 1873 K. It was found out that the CaO-CaF₂ system is close to the ideal solution. Structure of oxide-fluorides is topologically dense, total coordination number for Ca²⁺ ions changes from 5.2 to 6.8. The Ca-Me-O-F system (Me=Mg, Fe, Sr and Ba) was simulated by replacement of a few Ca²⁺ ions by the same number of Me²⁺ ions. Activity coefficients of MeO and MeF₂ solutes in the CaO-CaF₂ system were calculated and discussed in terms of basicity (acidity) of the solution. Analysis of MeO and MeF₂ activity coefficients in the CaO-CaF₂ system showed that with respect to MeO oxides, the CaO-CaF₂ system could be considered as a basic solution for CaO mole fraction above 0.8-0.9. At lower CaO concentration the CaO-CaF₂ system behaves as an acidic solution. With respect to MeF₂ solutes, the CaO-CaF₂ system may be regarded as a basic solution at about all compositions except the vicinity of pure CaF₂.

Finite element analysis of electromagnetically driven flow in sub-mold stirring of steel billets and slabs*T.T.NATARAJAN et al.*

This paper describes a new method for solving coupled three-dimensional electromagnetic and fluid flow equations in induction systems and its application to electromagnetic stirring in continuous casting of steel. This method is based on the differential-integral potential formulation of the electromagnetic field, and is capable of computing the field for any given stirrer configuration without solving the magnetic field in free space. The turbulent flow in the melt is represented by time averaged Navier-Stokes equation together with *k-ε* turbulent model. The finite element formulation of the governing equations are also presented. Computed results were presented for the electromagnetic forces, velocity and turbulent parameters in rotary stirring of billets and linear stirring of slabs during continuous casting of steel. For rotary stirring, it was found that the electromagnetic forces are confined to the region surrounded by the stirrer, and the effective flow region is about twice the length of the stirrer and exhibits weak axial velocity component. It was also found that the flow is turbulent with a maximum intensity of about 15% of the mean velocity, and decays rapidly above the edges of the inductor. For linear stirring of slabs, the spatial variation of the force field along and across the slab was found to generate a more complex flow pattern than

predicted by two-dimensional analysis. The turbulent field was found to increase monotonically in the direction of the traveling force field.

Decarburization kinetics of Fe-C-S droplets with H₂O*N.J.SIMONTO et al.*

Decarburization of liquid Fe-C-S droplets with H₂O vapour was investigated using the electromagnetic levitation technique. The results indicated that the decarburization of liquid iron droplets by H₂O vapour can be adequately described by the mixed control of the gas phase mass transport and the dissociative chemisorption of H₂O at the melt surface. The Steinberger-Treybal correlation equation was found to correctly represent the gas phase mass transfer in the present system geometry and experimental conditions. The rate of decarburization decreased significantly with increase in sulphur content in the melt, and this effect was quantitatively represented by the mixed control model. There exists a residual rate of decarburization at high sulphur contents in the melt. The extent of the residual rate observed can be interpreted as implying that, even at the melt surface of apparent saturation with sulphur, 8-9% of the surface sites are still available for H₂O molecules to react with carbon. The activation energy of dissociative chemisorption of H₂O was 95 kJ mol⁻¹.

Ironmaking and Reduction**Computational investigation of charging scrap to the blast furnace***P.R.AUSTIN et al.*

This paper examines the idea of using shredded scrap steel as a blast furnace burden material. Charging scrap, or metallics, with the burden offers several possible benefits including increased productivity and decreased fuel rate. In this paper, scrap charging is investigated numerically using a previously presented mathematical model. Furnace operations at both fixed hot metal temperature and fixed top gas temperature are investigated with scrap charged either near the axis, radially uniformly or near the wall. When the average temperature of metal entering the hearth is kept constant, the production and fuel rate are predicted to increase and decrease respectively as scrap feed rate increases. These changes are due to scrap being already fully reduced, thus not requiring heat or carbon for reduction. However, the top gas temperature decreases, particularly when scrap was charged only over the inner half radius of the furnace. Under conditions of constant top gas temperature the productivity and fuel still increase and decrease respectively with increasing scrap: ore ratio. Of the three scrap charging patterns tested, the optimum pattern is to charge scrap

over the outer half radius of the furnace, which results in the least change in the furnace internal state compared to operations without scrap while showing significant increases in production and decreases in fuel rate. Finally, scrap diameter is found to have only a small effect on the furnace state.

Casting and Solidification**Simple model for prediction of temperatures in an L-shaped tundish—Verification by continuous temperature measurements—***C.-E.GRIP*

A simple model concept developed for the SSAB steel plant was tested on data for another plant. That plant had an L-shaped tundish for billet casting. A special tanks in series model was developed for the steel flow in that tundish. The rest of the model could be used without change. It consists of simple equations for heat loss in ladle and tundish, as well as for the effect of thermal stratification and drainage flows in the ladle. The model was verified against existing data from continuous temperature measurements. The results show that the model approach developed for the steel plant of SSAB can also give good predictions with a different plant and tundish design. A simple mixing model could be used even for a complicated tundish configuration.

Modelling the eutectoid reaction in spheroidal graphite Fe-C-Si alloys*J.LACAZE et al.*

The so-called eutectoid reaction of spheroidal graphite cast irons (SGI) proceeds by competitive nucleation and growth of ferrite and pearlite. In the present study are first reviewed the physical models of the ferritic reaction in SGI previously described in the literature. Then, a new model is presented that uses a recent description of the conditions to be fulfilled for the ferritic and pearlitic reactions to start. This description is based upon the knowledge of the relevant phase diagram. Growth of the ferrite halos during the ferritic reaction is described as controlled by carbon transfer from the austenite/ferrite interface to the graphite nodules and by an interfacial reaction at the ferrite/graphite interface. Modelling of the pearlitic reaction accounts for nucleation of pearlite colonies, and their growth law is expressed according to experimental data available in the literature. It appeared also necessary to describe the diffusion of carbon in austenite before the beginning of the decomposition of this phase. Predictions are compared to experimental transformation kinetics obtained by means of differential thermal analysis on spheroidal graphite Fe-C-Si alloys, and could be easily extended to alloys with low level additions of pearlite promoter elements.

Mechanism of surface quality improvement in continuous cast slab with rectangular cold crucible mold

Y.-W. CHO *et al.*

The control of the initial stage of solidification for continuous casting of steel is extremely important in producing high surface quality products. The surface quality is strongly influenced by the oscillation mark on the solidifying shell, which could be improved by applying alternating electromagnetic field in the mold. A 50×200 mm rectangular cold crucible mold has been designed by numerical simulation and used for measuring the meniscus contour and local heating of molten metals using tin and lead. It has also been used in continuous casting experiment with Sn and Sn10%pb alloy to study the effects of frequency, input power, melt level in the mold, casting speed, mold cooling water flow rate, and mold oscillation frequency on the oscillation mark. The maximum melt temperature was observed near the triple point where the mold wall, melt free surface and the atmosphere meet all together. It has also been found that the local Joule heating density has strong influence on the oscillation mark formation.

Solute redistribution model of dendritic solidification considering diffusion both in the liquid phase and the solid phase

T. HIMEMIYA *et al.*

To estimate micro-segregation with dendritic solidification, a common method using an integral profile method has been developed. We considered three cases; (1) no diffusion in the solid and finite diffusion in the liquid, (2) finite diffusion in the solid and complete diffusion in the liquid, and (3) finite diffusion both in the solid and in the liquid. Expressing the solute distribution in the liquid and/or in the solid as quadratic polynomials, and assuming the linear growth case or the parabolic growth case, ordinary differential equations have been obtained. We introduced Ivantsov's solution as the initial condition of the diffusion problem to expand the model to rapid solidification conditions. Using the Runge-Kutta method, the solute distribution profile both in the liquid and in the solid over time was estimated. After calculation, good agreement with rigorous solutions for each case was gained. For easy way of programming and short computing time, this method has practical merits.

Surface Science and Technology

Effect of roll and rolling temperatures on sticking behavior of ferritic stainless steels

W. JIN *et al.*

The sticking behavior of several austenitic and ferritic stainless steels under the hot rolling conditions was examined in detail using a

two disk type hot rolling simulator. The sticking of bare metal to roll surfaces was strongly dependent on the high temperature tensile strength and the oxidation resistance of the stainless steel. A steel having higher tensile strength and lower oxidation resistance exhibited better resistance against sticking. The sticking occurred in increasing severity in the order of 430J1L, 436L, 430 and 409L. It was clarified that a high speed steel (HSS) roll was more beneficial to prevent sticking compared to a Hi-Cr roll.

Microstructure

Austenite grain growth behaviour of microalloyed Al-V-N and Al-V-Ti-N steels

N. GAO *et al.*

The austenite grain growth behaviour of microalloyed Al-V-N and Al-V-Ti-N steels has been studied. Estimations of austenite grain size for Al-V-N steels by several different grain growth inhibition models demonstrated that the best match to experimental results can be obtained from Gladman and Rios equations and it is AlN that controls the austenite grain size. The experimental and calculated results indicated that the drag force of plate-shaped AlN particles probably depends on their orientation and austenitising temperature. A modified Gladman model, which considers the effects of complex arrays of different types of particles on the stabilized austenite grain size, can be used to predict the austenite grain size and particle size for an Al-V-Ti-N steel when the combined effect of AlN and TiN is considered.

Modelling of the microstructure and the mechanical property variation across the transverse direction of hot rolled steels and the effect of edge shielding

J. K. LEE *et al.*

A computer-aided simulation model which can predict the temperature variation and the microstructural evolution in the process of hot rolling was developed by combining a metallurgical model and a thermal model. The developed model was utilized to analyze the variation of temperature and microstructure during hot rolling process and the mechanical properties of the final products across the transverse direction of a strip. The results of the simulation along with those of the mill trial tests indicated that the mechanical properties across the transverse direction were significantly influenced by the metallurgical in homogeneities developed in the stage of recrystallization and grain growth during rolling as well as the stage of transformation during cooling. In addition, the effect of the edge shielding during water cooling was quantitatively estimated by the present simulation model and the edge shielding was found to be effective in achieving uniform microstructure and mechanical properties in the hot rolled

steels, especially, steels with high hardenability.

Developments in macro and micro texture during plane strain channel die compression of IF steel

I. SAMAJDAR *et al.*

Textural developments in plane strain channel die compressed IF (interstitial free) steel were investigated for 7-75% reduction in thickness. Developments in macro texture were investigated by X-ray ODFs (orientation distribution functions) and were simulated by Taylor type models, while actual microtextural developments were studied by OIM (orientation imaging microscopy). Although a gradual increase in α -fiber (RD// $\langle 110 \rangle$) was observed with increased reductions, γ -fiber (ND// $\langle 111 \rangle$) increased till 40-50% reduction and then remained almost the same. At the earlier stages of deformation and in general for relatively larger grains, areas around grain boundaries were relatively more deformed (*i.e.* with more frequent low angle boundaries) and more rotated (as tested in split samples at 7 and 18% reduction) than the grain interior. Till 50% reduction, deformation substructures among deformed grains of different orientations were not significantly different. Above 50% deformation, relatively intense strain localizations (in the form of higher frequencies and larger misorientations of grain boundaries) were observed to form at an angle of about $\approx 37^\circ$ with RD (rolling direction), somewhat more preferentially in the γ -fiber deformed grains of F $\{111\}\langle 112 \rangle$ and E $\{111\}\langle 110 \rangle$ components. The appearance of such strain localizations increased the stored energies of F/E bands and also possibly accounted for the formation of new high angle boundaries (as evident from increased grain splitting factors).

Continuous cooling transformation behaviour of high strength microalloyed steels for linepipe applications

P. A. MANOHAR *et al.*

Continuous cooling transformation (CCT) behaviour of high strength microalloyed steels containing two different levels of Mn+Si additions is investigated in undeformed and thermomechanically processed conditions using quench and deformation dilatometry respectively. The deformation schedule used in the dilatometer is designed to simulate the industrial controlled rolling procedures for the production of plates as closely as possible in laboratory. CCT diagrams for the undeformed and thermomechanically processed steels are constructed. Effects of thermomechanical processing (TMP), accelerated cooling and composition (Mn+Si levels) on γ transformation start temperature (Ar_3), phase transformation kinetics, CCT diagrams and microhardness are investigated.

The results show that TMP accelerates the onset of γ/α transformation (Ar_3 is raised), but

the progress of γ/α transformation is retarded considerably in deformed samples. Significant retardation is observed during the final 30 % of the phase transformation reaction. Increase in cooling rate lowers the Ar_3 significantly and accelerates the progress of transformation. The steel with a higher level of Mn+Si addi-

tion (1.96 %) exhibits lower Ar_3 , sluggish transformation kinetics and higher hardnesses in undeformed and thermomechanically processed conditions as compared with the steel with a lower level of Mn+Si addition (1.17 %). These effects are explained in terms of the effects of Mn and Si contents on the carbon

partitioning and the subsequent phase transformation behaviour of these steels during continuous cooling. Increase in cooling rate increases the microhardnesses of both steels while TMP lowers them.