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BOOK OF ABSTRACTS

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Controlled directionality in 3D printing of graphite-reinforced polymer composite with enhanced mechanical properties

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Abstract

In the realm of additive manufacturing (AM) for polymer composites, the precise control of reinforcement orientation, distribution, and porosity plays a pivotal role in determining mechanical properties. This study focuses on manipulating printing conditions, such as nozzle diameter and flow rates, to achieve optimal reinforcement alignment within the printed structure. By varying these parameters, researchers aim to enhance mechanical performance compared to traditional methods like film casting. Experimental observations underscore a direct relationship between the orientation of reinforcement fibers, resultant porosity levels, and the mechanical strength of the composite. For instance, the 3D printed composites demonstrated substantial improvements: approximately 108% higher tensile strength, 520% greater toughness, and a notable 188% increase in fracture strain compared to conventionally cast films. These enhancements highlight the efficacy of AM in tailoring material properties through controlled reinforcement alignment.

To further elucidate and validate these experimental findings, the study employs advanced computational modeling techniques. Specifically, the combination of Discrete Element Method (DEM) and Computational Fluid Dynamics (CFD) provides insights into the intricate dynamics of particle alignment within the extrusion nozzle. This approach allows researchers to simulate and visualize how varying printing parameters influence the spatial arrangement and orientation of the reinforcement particles during the manufacturing process. Graphite particles, chosen for their reinforcing capabilities, are embedded within a polyvinyl alcohol (PVA) matrix. The study investigates different weight percentages of graphite and conducts rheological tests to characterize the ink's viscosity and flow behavior. This thorough examination ensures that the ink remains extrudable through nozzles of different diameters (ranging from 0.7 to 1.4 mm), crucial for achieving desired reinforcement alignment and overall print quality. The computational models, implemented using software like Rocky 4.5.2 for DEM and Ansys Fluent 2021 R1 for CFD, not only validate experimental results but also offer predictive capabilities. By tracking individual particle movements and interactions, these simulations predict parameters such as particle distribution, average inter-particle distance, porosity levels, and mechanical performance metrics. Moreover, through multi-regression analysis, the study establishes mathematical models that correlate input variables (printing conditions) with output variables (composite properties), facilitating future optimizations in AM processes.

Key words: CFD-DEM, 3D printing, additive manufacturing, polymer composites

Kinetics of the reaction between solid inclusions in liquid steel

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Abstract

Calcium treatment in steel production is commonly used to modify solid alumina or spinel inclusions into more desirable liquid or partially liquid calcium aluminates or calcium magnesium aluminates. The reaction of dissolved calcium or its vapor with pre-existing alumina inclusions, resulting in their modification, is commonly known as direct modification. Transient inclusions such as CaS or CaO can also form during calcium treatment, depending on the levels of sulfur or oxygen dissolved in the liquid steel. Research indicates that these transient inclusions, CaS or CaO, physically interact with and chemically react to the existing alumina inclusions, ultimately modifying them into calcium aluminates. This route of modification is known as indirect modification. However, the kinetics of these reactions between solid inclusions in liquid steel in indirect modification have not been documented in the literature.

The calcium transfer from CaS or CaO inclusions to alumina or spinel inclusions is expected to occur via calcium dissolution in liquid steel. For small inclusions (<5 μm), the rate of reaction is expected to be limited by mass transport from the bulk of the liquid steel to the steel-inclusion interface. A kinetic model is developed considering the mass transport rates and local thermodynamic conditions to calculate the rate of calcium modification via indirect mode. The model couples FactSage thermodynamic calculation to a program written in C using ChemApp. The calculation suggests that in the presence of CaS and Al_2O_3 inclusions, the rate of transport of calcium and oxygen through the bulk steel is expected to determine the rate of inclusion modification.

Keywords: Nonmetallic inclusions, Transient inclusions, Inclusion modification, Kinetic Model

Prediction of leaching efficiency of Rare Earth Elements (REEs) from Phosphogypsum by machine learning methods

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Abstract

Rare Earth Elements (REEs) are a group of 17 elements consisting of 15 Lanthanides, Yttrium and Scandium. These elements have extensive applications in many strategic domains like renewable energy, defence, and electronics. Since most of the global demand for REEs is catered by China, there is an urgent need to extract these critical elements by other nations from secondary sources. One such source is phosphogypsum (PG), which is an industrial by-product of the phosphoric acid manufacturing process. Conventionally, researchers have used hydrometallurgical techniques like leaching and solvent extraction to extract these valuable metals from PG. Most of the leaching studies reported in literature are based on leaching of PG with mineral acids like sulphuric acid, nitric acid and hydrochloric acid. Hence, in the present work, two machine learning algorithms (XGBoost (XGB) and Random Forest Regressor (RFR)) are used to predict the leaching efficiency of REEs from phosphogypsum. The models were trained and tested on an exhaustive dataset built based on reported literature data. Four process parameters, namely, temperature, acid concentration, solid-liquid Ratio, and process duration, were taken as inputs to predict the leaching efficiency of REEs. The K-Fold cross-validation showed that XGBoost is a better model than RFR with 81.4% accuracy and 6.5% standard deviation. Further, leaching experiments were performed with commercially available phosphogypsum sample with sulphuric acid and nitric acid as lixiviants. The concentration of REEs in PG sample used in this study is 420 ppm. In general, the XGBoost model predictions showed good agreement with the experimental results. The highest leaching efficiency achieved experimentally for sulphuric acid and nitric acid was 50% and 70%, respectively, for which the corresponding ML predicted leaching efficiencies were 39% for sulphuric acid and 72% for nitric acid.

Keywords: Rare Earth Elements, Phosphogypsum, Machine Learning

Exploring Slag Foaming and Flushing Dynamics in EAF Steelmaking: Insights from a Cold Model Study

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Abstract

Electric Arc Furnace (EAF) steelmaking is a complex process involving melting and refining of raw materials through arcing and adding suitable flux and additives. Slag foaming is often employed for efficient melting and enhancing equipment life. EAF can handle a variety of iron-bearing charge materials such as scrap, direct reduced iron (DRI), hot metal in different proportions, and fluxing materials like lime and dolomite. Depending on the charge materials and furnace design, additives in the furnace can have varying proportions of carbon, oxygen, and flux materials such as lime and dolomite. EAF operation under consideration involves scrap, DRI, and hot metal as charge materials and carbon, oxygen, lime, and dolomite as additives. Owing to the high volume of slag generated and slag foaming, there is a continuous discharge (flushing) of slag throughout the heat. With the progress of heat, slag temperature and chemistry change dynamically. Also, DRI, lime, and dolomite are added continuously to the vessel. These materials contribute to the slag formation and refining through slag-metal reactions. However, these additions also contribute to undissolved particles in the slag. Under these conditions, slag foaming and flushing behavior become challenging. To understand the slag foaming and flushing behaviour under the impact of undissolved particles, a cold model setup was developed. Silicone oil and paraffin wax were used to simulate liquid slag and solid particles, respectively, in a two-phase mixture. Gas was generated using an air compressor and uniformly distributed via a quartz-fitted disk with a 15-40 µm porosity. The viscosities of pure liquid oils and the solid-liquid mixtures were measured using a Rheometer (Anton Paar MCR102), and the density of the oil was determined to be approximately 960 kg/m^3. The study revealed significant insights into the effects of the proportion of the solid particle on slag foaming behavior. It was also observed that even when the viscosities of pure liquid and liquid-solid mixtures were comparable, the slag foaming characteristics were different. Additionally, the slag flushing phenomenon did not exhibit a linear relationship with the gas generation rate and the viscosity of the two-phase mixture, highlighting the complexity of the process. This work provides valuable insights into the dynamics of slag formation, foaming, and flushing, which are critical for improving EAF operational efficiency and productivity. The key findings from this research will be presented.

Keywords: Electric Arc Furnace (EAF), DRI, Cold Model Experiment, Slag Foaming, Two-Phase Mixture, Viscosity Measurement

Mathematical Modeling of Motion of Carrier Gas and Mg Particle in the Top Lance during Hot Metal Desulphurization Process

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Abstract

The desulphurization (DeS) reaction efficiency in the hot metal (HM) bath mostly depends on the Mg bubble-hot metal interactions. The behavior of gas and particles in the external DeS unit top-lance has been investigated. In the present work, different forces acting on the Mg particle and carrier gas while traveling in the lance and into the hot metal bath have been studied using a mathematical model. The newly developed mathematical model accounts for forces like the effect of lance-wall drag and pressure loss at the bend of the T-shaped nozzle, in addition to the conventional forces. The effect of lance geometry has been taken care of by considering various types of cross-sectional lances, such as circular, ellipse, pentagon, and hexagonal-shaped lances. Moreover, composite heat transfer from the HM to the particle is studied considering the skull formation/dissolution on the outer surface of the lance immersed in the bath. The results include estimating the temperature profile from the liquid bath through the skull layer, refractory shell, steel pipe, and carrier gas to the Mg particle. Subsequently, the temperature & velocity of gas and solid Mg particles inside the lance have also been calculated. In addition, penetrability analysis for the gas jet at the lance tip and the behavior of the Mg particles has been investigated. The results from the developed model can be utilized to design a lance for the physical model, and subsequent results can be validated in the future.

Keywords: Hot metal, Desulphurization, lance, Penetrability, mathematical model

Insights into thermomechanical processing of Al added low density medium Mn steel

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Abstract

In this study, the Al (~3 wt%) added low density medium Mn steel has been developed by melting-casting route in an open-air induction furnance. The cast ingot has been hot forged and hot rolled to 50% thickness reduction in temperature range of 1100-800°C after soaking at 1100 °C for 2 hrs. After hot rolling, two different cooling mediums, still air and water quenching has been chosen to cool to room temperature. Subsequently, the rolled samples has been intercritical annealed at 720°C for 1 hr and then air cooled to room temperature. The phase fraction of specimen after every thermomechanical processing has been analyzed by rietveld refinement using X-ray diffraction (XRD) peaks. The microstructure characterization has been carried out by using optical microscopy, scanning electron microscopy, electron back scattered diffraction and transmission electron microscopy, and 3D atom probe microscope. The microstructural analysis shows the formation of multiphase microstructure of elongated ferrite and lamellar structure of martensite + austenite in hot rolled as well as annealed condition. The xrd analysis reveal that the austenite fraction in intercritical annealed sample has significantly increased compare to hot forging and rolling due to elemental partitioning during annealing. However, the highest fraction of austenite has been found in the annealed sample that is water quenched compare to air cooled after hot rolling. Therefore, it shows the highest total elongation of 40±2.5% with yield strength and ultimate tensile strength of 593±10 and 854±20 MPa respectively due to the presence of high fraction of reversed austenite with suitable mechanical stability. The annealed sample that is air cooled after hot rolling possesses the ultimate tensile strength, yield strength and ductility of 1000±20 MPa,700±10 MPa and 18.5 ± 0.5, respectively. Interestingly, it also reveals the precipitation of kappa (k) carbide in intergranular region may be due to segregation of C and Al. The xrd analysis of annealed sample (before tensile test) shows both ferrite/martensite and austenite peaks, whereas after tensile test, it represents mainly ferrite/martensite peaks. This shows the enhanced transformation-induced plasticity (TRIP) effect during tensile test. The TEM analysis of annealed sample (before tensile test) and after tensile test also confirm the occurrence of TRIP effect during tensile loading. Moreover, the stacking fault energy (SFE) of the steel has been found to be ∼16 mJ m^{-2}, calculated by the modified Olson and Cohen method too concludes TRIP is the preferred deformation mechanism in the developed steel.

Key words: Al added low density medium Mn steel; Thermomechanical processing; Kappa (k) carbide; Microstructural evolution; Tensile properties

Effect of variation of composition on atomistic structure of ternary Cu – Zr – Al based BMG

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Abstract

Bulk metallic glasses (BMGs) are known for their exceptional strength and corrosion resistance. They are used for critical structural applications and biomedical engineering. The glass-forming ability (GFA) of elements is considered while making BMGs. A combination of Cu, Zr, and Al are found to have excellent GFA and therefore are used for making BMGs. It has been observed that by altering composition and optimizing cooling rate, stable structures, and improved mechanical properties can be achieved. In this work, a ternary Cu – Zr – Al-based BMG is taken into consideration and the impact of varying composition on the amorphous structure of BMG is studied. The presence of Full Icosahedra (FI) clusters in BMGs promotes the stability of the glassy amorphous structure and indicates better GFA. Molecular dynamics-based modeling and simulation have been carried out to have an atomistic insight-based detailed analysis on the variation of composition on the formation of FI clusters. In general, a total of 36 samples have been taken into consideration by ranging Zr from 40 at % to 60 at. % with step size of 4 and Al from 5 at. % to 10 at. % with a step size of 1. Initially, glass transition temperatures (Tg) are determined, and then annealing is carried up to 0.9Tg to determine the number of FI clusters in the system.
It has been observed that by keeping the cooling rate at 10^{11} K/s, the number of FI clusters increases with an increase in Al whereas the number decreases with an increase in Zr or a decrease in Cu. This gives valuable insights about the stability of BMGs.

Keywords: Full icosahedra, Glass forming ability, Glass transition temperature, Molecular Dynamics

Fluid flow and heat transfer during injection molding of PET

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Abstract

Injection molding, a most common processing method for thermoplastics, is a cyclic replication-based molding process ideally suited to produce mass components with extreme repeatability. The thermo-mechanical conditions inside the cavity affect the morphology and properties of the final component, with thermal contact resistance (TCR) at the polymer/mold interface being a critical factor.

A 16 kN pneumatically operated vertical injection molding machine (experimental setup) was designed and fabricated to estimate polymer/mold interfacial heat flux transients during the cyclic process. The PET (Poly Ethylene Terephthalate) melt from the heated barrel is injected into the mold cavity under pressure. The mold filling time, velocity, and shear rate profiles of the melt were assessed by the time delay in the response of the adjacent K-type thermocouples placed in line with the melt flow direction. Experiments were conducted at a melt injection temperature of 280°C and the maximum shear rate at the wall during mold filling was found to be 45 s^{-1}. The study also examined the wettability of polyethylene terephthalate (PET) melt on steel substrates, considering surface roughness and temperature. Contact angle measurements showed temperature had a greater impact on wetting than roughness. Surface free energy of steel decreased by 22% as roughness increased from 0.21 µm to 3.8 µm. After the filling stage, the melt cools down to the ejection temperature by rejecting heat to the mold. By utilizing the recorded temperature history of the mold, an inverse heat conduction problem (IHCP) was adopted to estimate the spatio-temporal heat flux transients at polymer/mold interface and thus the mold surface temperature. The interfacial heat flux transients were then used to simulate the cooling behavior of the polymer melt. The peak heat transfer coefficient (HTC) was found to be 5775 W/m^2K at a dimensionless interface temperature ratio of 0.75. The air gap at the interface evolved with an exponential fit, starting at 4 µm at peak HTC and increasing to about 100 µm by the end of solidification. Peak heat flux corresponded with polymer skin formation on the mold, while peak HTC marked the start of air gap nucleation. Accurate HTC values are essential for reliable simulation of the temperature distribution in the solidifying part, as incorrect values can lead to defects.

Cooling rates affected the opacity of solidified PET melt, quantified by image analysis in MATLAB. Opacity declined sharply at lower cooling rates before stabilizing at higher rates, with three solidification regimes identified: increased crystallization at cooling rates below 8°C/min, amorphous characteristics at rates above 199°C/min, and a transitional regime at intermediate rates. No significant difference in mean pixel intensity was observed between PET melts solidified at different substrate temperatures.

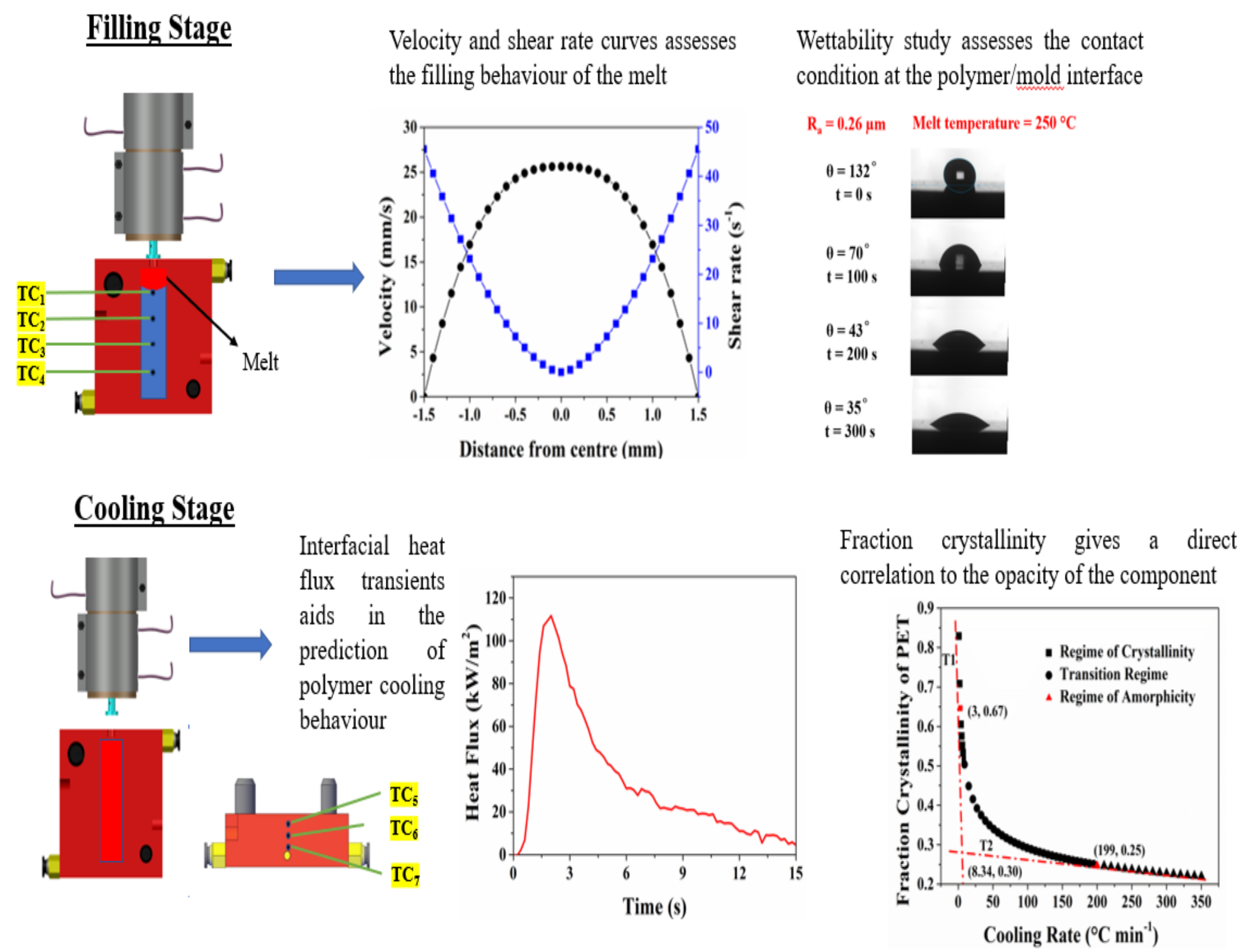

Fig. 1 Graphical representation of the fluid flow and heat transfer during injection molding of PET.

Key words: injection molding; shear rate; wettability; heat flux transients; crystallinity; amorphicity; cooling ra

Layered intercalated architecture of Ni2V2O7 nanoparticle and N-doped reduced graphene oxide composite sheet as an electrode material for asymmetric supercapacitor

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Abstract

The depletion of fossil fuels and the environmental impact of greenhouse gas emissions have increased the global demand for sustainable energy sources. Renewable energies like wind, hydro, and solar have helped reduce ecological damage, but efficient storage is crucial for future use. Research has focused on eco-friendly energy storage solutions, with supercapacitors gaining attention for their high power density, fast charge-discharge cycles, and long lifespan, making them ideal for future electronic devices. Recently, there has been a preference for using metal oxides with carbon-based substances, including activated carbon, graphene, and carbon nanotubes (CNT). The reason for this choice is their excellent larger surface area and electrical conductivity. The novelties of the present work are to demonstrate enhanced electrochemical performance by the incorporation of varying weight percentages of nitrogen-doped reduced graphene oxide (N-rGO) into the $Ni_2V_2O_7$ (NVO) electrode material. To our knowledge, the incorporation of N-rGO into the NVO electrode material has not been yet reported. This study presents NVO nanoparticles integrated within an N-rGO layered structure, serving as a positive electrode material for supercapacitor applications. The composite is synthesized using an inexpensive and easily scalable route of the hydrothermal method. Among the as-synthesized N-rGO-NVO composites, the 40 wt% N-rGO-NVO composite delivers excellent electrochemical performance. It delivered a specific capacitance of 712.5 F g^{-1} at 1 mA cm^{-2} fixed current density. An asymmetric supercapacitor (ASC) energy storage device was fabricated utilizing the 40 wt% N-rGO-NVO composite material as the positive electrode while the negative electrode is made from activated carbon (AC). The fabricated ASC device displays an energy density and power density of 14 Wh/kg and 7500 W/kg at 10 mA cm^{-2} current density. The fabricated ASC device maintains about 75% of its original capacitance retention after undergoing 5000 cycles of charge and discharge at 10 mA cm^{-2} current density.

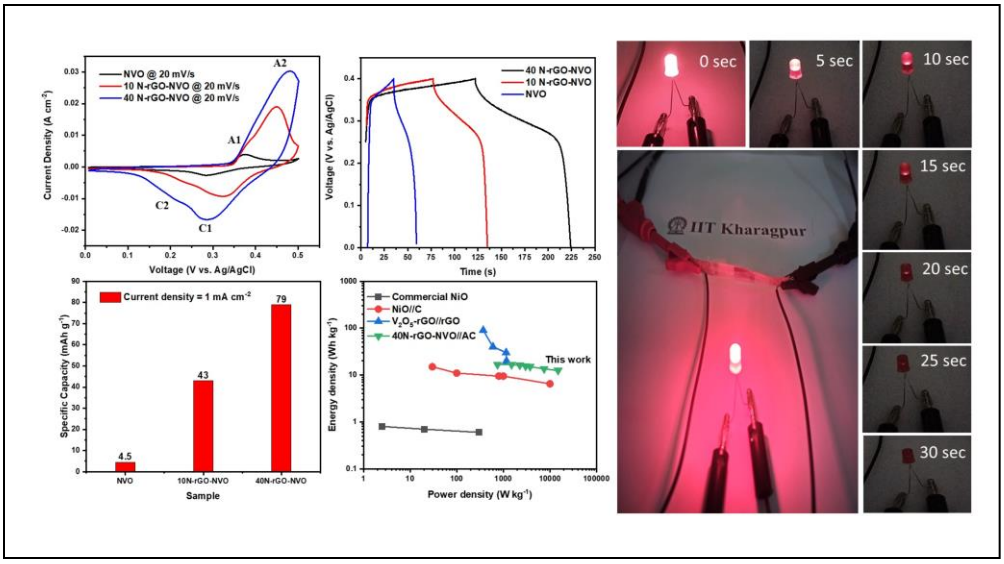

Figure 1: Fabrication of asymmetric supercapacitor using 40N-rGO-NVO positive electrode material.

Keywords: $Ni_2V_2O_7$, layered intercalated architecture, asymmetric supercapacitor, electrochemical energy storage

The influence of CaF2-freeSAW fluxes on the elemental transfer behavior: Thermo-chemical modeling approach

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Abstract

CaF_2 has traditionally been an essential constituent in fluxes used for Submerged Arc Welding (SAW) of steel plates. The widespread use of CaF_2in these fluxes is driven by its ability to lower the liquidus temperature and viscosity of the molten slag layer, as well as its contribution towards control over the total oxygen (O_{total}) content in the weld. However, environmental and health hazards arising from evaporation of fluoride vapour from the molten slag is prompting researchers to aim at replacing CaF_2 with more benign constituents. With this guiding objective in mind, "alternate" CaO-SiO_2-Al_2O_3-MnO compositions were identified for potential use as SAW flux, without compromising on the thermo-physical properties required for submerged arc welding of low carbon steel.[1] These "alternate" fluxes were benchmarked with commercially used SAW fluxes, to establish their suitability for the application. In the present work, chemical compositions of the base plate, welding electrode, weld metal as well as the slag formed were analysed to establish the nature of element transfer between the weld metal and molten flux. The welding process was simulated through a Thermo-chemical model based on FactSage™ macros, using the Effective Equilibrium Reaction Zone (EERZ) approach. The simulations were validated with the measured chemical analyses of the weld metal and the slag layer. The results from the simulations were helpful to understand the transfer of solute elements like Si, Mn, Al and O between the different phases in the weld zone. The importance of this knowledge lies in the influence exerted by these elements on the fracture toughness to the welded joint. The simulations involving gas-slag-metal reactions could reasonably predict the transfer of solute elements under the situation of using the CaF_2-free alternate fluxes.[2]Concentration of Si, Mn and Total O were reasonably close to the values measured in welds carried out using conventional fluxes. This approach is expected to reduce the dependence on time and resource-consuming welding trials.

Keywords: Welding flux, FactSage™ simulations, Steel

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Interparticle Diffusion Kinetics of Reduction of Hematite Fines by Hydrogen at Moderate Temperatures

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Abstract

In many metallurgical processes, the reaction between an initially nonporous solid and a gas produces a porous solid product. Thereafter, the reaction rate can be controlled by either the interfacial reaction or interparticle diffusion, or both. making both chemical kinetics and interparticle diffusion crucial factors. In such cases, obtaining closed-form rate expressions for conversion versus time becomes challenging and the "law of additive reaction times" can be conveniently used for determining the overall reaction rate. This law states that the time required to attain a certain conversion is the sum of the time required to reach that conversion in the absence of interparticle diffusion and the time required to reach the same conversion under the control of the interparticle diffusion. In a previous investigation, intrinsic kinetics of hematite reduction by hydrogen was determined using a thin layer of hematite ore fines to eliminate the diffusional effect. The present work is carried out to investigate the reduction of hematite ore fines when the reaction is governed primarily by interparticle diffusion. The influence of reduction temperature, particle size (56, 112 and 181μm) and bed height (0.5-1.5 cm) on the reaction rate is examined. Chemical composition and phase changes of hematite fines before and after reduction were carried out using XRF, XRD, and EDS-SEM. The effective diffusivity was determined using a mathematical model fitting approach for different particle sizes at various temperatures. It was found that an increase in the reduction temperature increased the diffusivity coefficient. The experimental results also showed that time required to achieve certain conversion is proportional to the square of bed height. The apparent activation energy of different particle sizes was found to be ~33.5 kJ/mole in a global step ($Fe_2O_3 \rightarrow Fe$).

Keywords: Interparticle diffusion, Hydrogen, Hematite ore fines, Reduction temperature.

Innovative Approach for Transforming Iron-Rich Electric Arc Furnace Slag into a Secondary Resource for the Steel Industry

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Abstract

Steel industries are a major value-added source worldwide, accounting for 3.8% of global GDP. One of the most pressing issues facing by the steel industry is management of large amounts of solid waste, such as steel slag. Steel slag is formed as a by-product of steelmaking processes when impurities are separated from molten steel in steel-making furnace. Steel slag production accounts for 10% to 15% of total global steel production, or 188.82 MT to 283.23 MT in 2023. In which 30% of steel slag is produced via. the DRI-EAF route, which is expected to increase as steel industries work to decarburize their products. This slag contains a high concentration of iron, calcium, silica, and other minor elements. The presence of a large amount of iron in slag limits its use for various construction and other landfilling applications, which are also not economically and environmentally beneficial. Therefore, post-treatment of slag is required to extract the iron from the complex slag structure before it can be used in potential application.
This study investigated DRI-EAF slag to turn waste into valuable and sustainable feedstock for steelmaking with nominal operational cost and high environmental impact. The process proceeds by utilizing latent heat in molten slag, molten-stage reduction, optimization process condition, specific energy consumption, and viscosity-driven separation between iron and slag. The significant reduction of iron oxides in the slag was seen at up to 73.4% to 83.34% at 1600°C in starting 15 minutes. About 97.8% of iron recovery was obtained under optimum conditions: basicity 1.2, carbon/oxygen ratio 1, and reduction time 40 minutes. The iron-slag separation mechanism found one of the important parameter during this study. The settling velocity of iron particles at molten stage got decrease with increasing slag basicity, reaching values of 3.13×10^{-5} m/s, 1.95×10^{-5} m/s, and 0.89×10^{-5} m/s for slag basicity 0.9, 1.2, and 1.5, respectively. The effects of slag basicity on slag viscosity, phase formation, and energy consumption are thoroughly investigated. This finding potentially contributes to managing the DRI-EAF steel slag treatment for producing steel-based products and reducing associated pollution.

Keywords: Recycling, Iron Reduction, Metal Separation, Slag Valorization.