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IIM METAL NEWS

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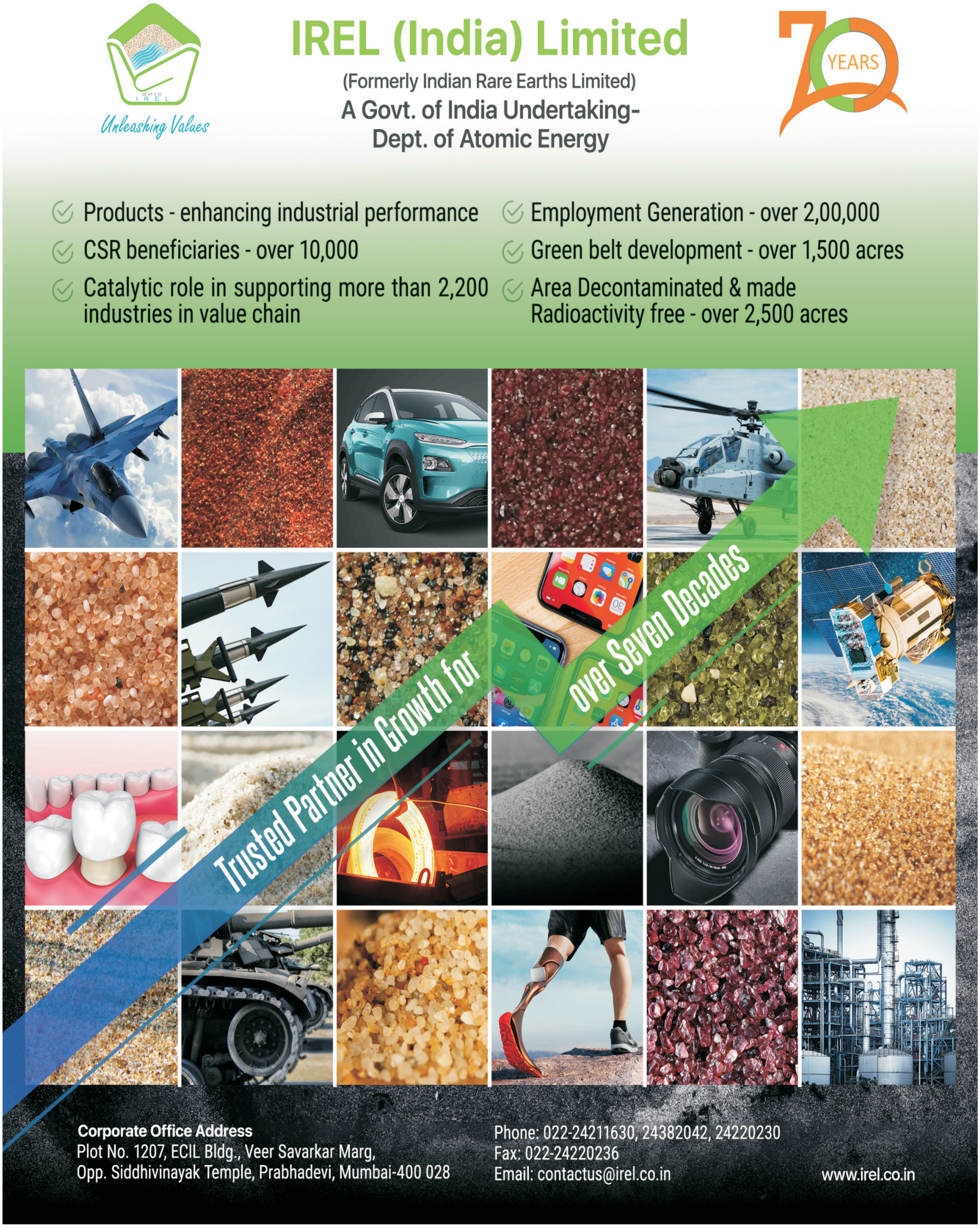
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IIM METAL NEWS

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Technical Article

A Multi-Scale Modelling Approach for Engineering Realization of a Casting Component

Ujjal Tewary[1], Goutam Mohapatra[1], Shyamprasad Karagadde[2], Alankar Alankar[2], Indradev Samajdar[3], Satyam S Sahay[1]

Abstract

In a traditional engineering component development workflow, design, process modelling and virtual performance evaluation and verification are considered to obtain a robust engineering component. In this approach, material is assumed to be continuum, having homogeneous material properties throughout the component geometry. However, such an assumption constraint achieving optimal component design. In this study, the traditional engineering component development workflow was modified by adding a multi-scale (macro, meso, micro, and nano) material model. At the macro-scale, thermal models were developed to simulate the casting process. At the meso- and micro-scale microstructure models were developed to predict microstructural features based on the information obtained from the higher (macro) and much lower (nano) lengths and time scales. Finally, constitutive models were developed based on the microstructural features to predict bulk and local deformation behaviour. Experiments were performed at various length-scale to obtain input parameters for the multi-scale models and to validate the models' predictions. An industrial implementation strategy for the modified workflow is discussed for an actual tractor casting component. It is envisaged that the framework and higher fidelity models proposed in this study will help to better design and obtain a robust and optimized engineering component.

Keywords : Cast iron, Graphite morphology, Microstructure, Mechanical behaviour, Multiscale modelling.

1. Introduction

Cast iron is an important engineering material. It is a preferred material for transmission housing, axle blocks, and engine components in automobiles and off-highway vehicles [1]. Often, it is an alternate material choice for welded structures where the weldment location has a performance issue. The major advantage of using cast iron is that it enables manipulation and optimization of the local geometrical thickness of components to achieve optimum mass. It is also a very flexible material as the microstructure and consequently, properties can be tailor-made, with a change in composition [2,3] and thickness [4,5] of casting geometry. Graphite morphology, an important microstructural constituent, can be changed from flakes to compacted to spheroidal based on magnesium (Mg) treatment [2], while the matrix microstructure can be ferrite, pearlite, or martensite [3].

There are several steps involved in the engineering realization of a casting component during component development. Fig. 1a shows the traditional component development workflow. To obtain a robust component, the workflow starts with concept development. This is followed by component design, process modelling and virtual performance evaluation and verification cycle. This cycle often is an iterative process until a robust component is designed and evaluated. In component design, computer-aided design (CAD) has unanimously become an accepted way to design a component. Whereas in the process modelling, simulations are often carried out using MAGMASOFT®, ProCast® or equivalent software to simulate the casting

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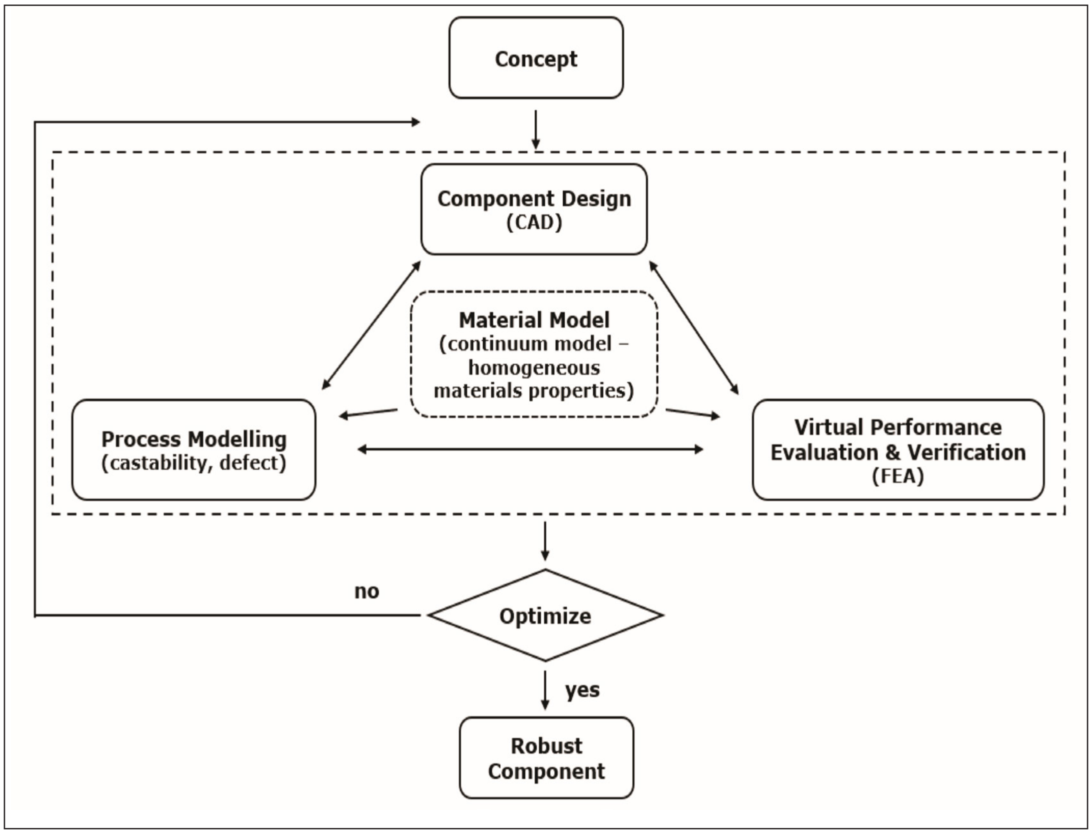
process to obtain an optimized design with zero defect [6]. In the virtual performance evaluation and verification step, the component (geometry/shape and material) interacts with the environment regarding applied loads, boundary conditions, and suitable atmosphere. These factors form the inputs into the computational model. The finite element method (FEM) has won acceptance as a tool to solve a mathematical model, which is very complex and for which analytical solution techniques are generally not possible. Traditionally, the continuum-based finite element material model is widely used which often does their purpose quite well. In this method, a material is homogeneous, having uniform properties throughout the geometry.

Owing to the stringent emission norms, there is an increasing drive towards designing light-weight engineering component without sacrificing performance requirements. This entails a higher fidelity approach. In this context, multi-scale modelling bridges this gap. In this approach instead of a continuum-based material model, microstructure and microstructure-informed constitutive models are to be considered. These higher fidelity models are to be integrated with the process modelling and virtual performance and verification modelling workflow (see Fig. 1b and section 4) to obtain better performance predictions and a highly robust and optimized component.

In this study, a multi-scale approach involving modelling and experiments was developed for microstructure and mechanical property predictions and validated for different types of cast irons – grey cast iron (GCI), compacted graphite cast iron (CGI), and spheroidal graphite cast iron (SGI). In section 2 of this manuscript, a succinct description of the approach has been delineated. In section 3, a few key results from the multi-scale model and its validation with experiments are provided and discussed. In section 4, an industrial implementation strategy of the approach for the component development workflow and its implication has been discussed. Finally, in section 5, the whole approach has been summarized along with a few key challenges for applying this framework to the industries.



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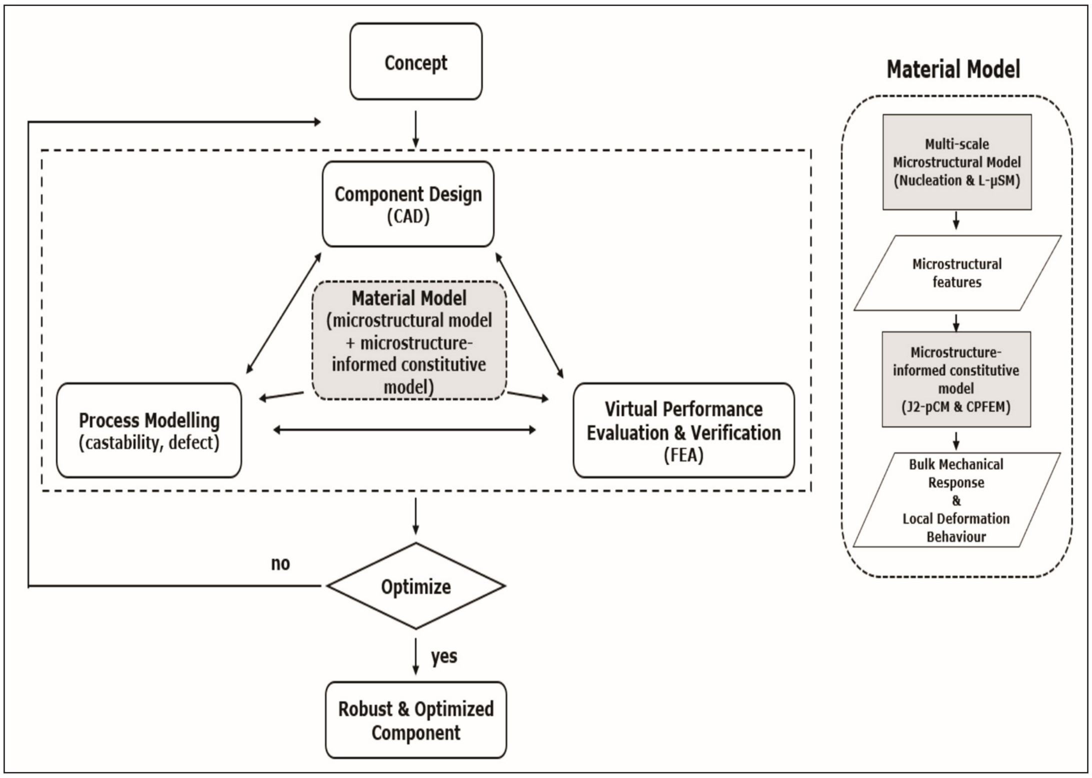


(b)

Fig. 1 : (a) Traditonal engineering component development workflow where component design, process modelling and virtual performance evaluation and verification are considered iteratively to obtain a robust component. Here material is a continuum, having homogeneous material properties throughout the geometry, (b) Proposed engineering component development workflow. Here microstructural models and microstructure-informed constitutive models are being considered instead of homogeneous material properties throughout the geometry. Alongside this, a detailed description of the material model was provided, which involves a multi-scale microstructural and microstructure-informed constitutive model.

2. Multiscale Modelling and Experimental Approach

A finite element-based multi-scale model was developed to simulate the casting of different types of cast irons. Fig. 2 shows the overall framework, both modelling and experimental. In this framework, the casting geometry was discretized into several elements. Each element in the geometry comprised a set of Gaussian Integration points (NPT), each represented by a representative volume element (RVE) where the macroscopic heat balance equation (thermal model) was solved (see Fig. 2). Temperature and time were outputs from the macroscopic thermal model. In each RVE, nucleation of graphite during solidification (microstructural model) was modelled. Each RVE were further discretized into smaller elementary volumes (meso-scale). The number of graphite particles (nucleated) decided the number of elementary volumes in each RVE. The growth of graphite was modelled at a lower length scale (micro-scale) using a Lagrangian-based micro-scale model (L-μSM). In the L-μSM, a unified graphite growth analytical model was developed based on the interfacial free energy, Mg concentration in the vicinity of a growing graphite, and graphite orientation [2,7]. The interfacial free energy was computed using molecular dynamics (MD) simulation at the nano-scale based on the elemental segregation (particularly Mg) measured using Auger Electron Spectroscopy (AES) [2]. Graphite orientation was measured experimentally by Electron Backscatter Diffraction (EBSD) in a Scanning Electron Microscopy (SEM) [2].

The predictions from the microstructural model (both at micro-scale and meso-scale) were on the cooling curves (time-temperature) during the solidification process and on microstructural features like graphite number density, size of graphite particles, shape of graphite particles, and volume fraction of phases (see later). A Python script was developed to obtain two-dimensional micrographs from the microstructural numerical models (both micro-scale and meso-scale). This was validated with optical microscopy experimental results. The microstructural features, like graphite number density, graphite size and graphite shape, were averaged to obtain information at a macro-scale, which was validated with three-dimensional X-ray microscopy (3D XRM) experimental data. The predictions on cooling curves for different types of casting of cast irons were validated with time-temperature experimental data captured using thermocouples during the casting process [2,4,7].

Two constitutive models were developed to study the bulk mechanical response and local deformation behaviour of cast irons – (1) J2 plasticity constitutive model (J2-pCM), and (2) crystal plasticity finite element-based model (CPFEM). The J2-pCM model is based on the von Mises criteria, that is, plastic deformation occurs when the effective plastic stress reaches the von Mises stress of the material or phases. The J2-pCM was integrated into a finite element modelling framework to predict the local and bulk stress-strain behaviour based on the morphology of the graphite phase. Moreover, a higher-fidelity CPFE model was developed. The CPFE is based on the principles that on the application of stress (or strain) to a material, a single or polycrystal will respond to the applied stress by dislocation slip. The applied stress will also reorient the grains during deformation. At the same time, the threshold stress of each slip system will increase because of self-hardening and latent hardening of the deformation modes. The predictions from the CPFEM were on a bulk mechanical response (stress-strain curve), local deformation response, and the orientation of the crystals (that is, texture). The bulk mechanical response of cast irons was validated with Gleeble tests, and local deformation behaviour was validated with *in situ* Digital Image Correlation (DIC) and EBSD measurements in the SEM setup.

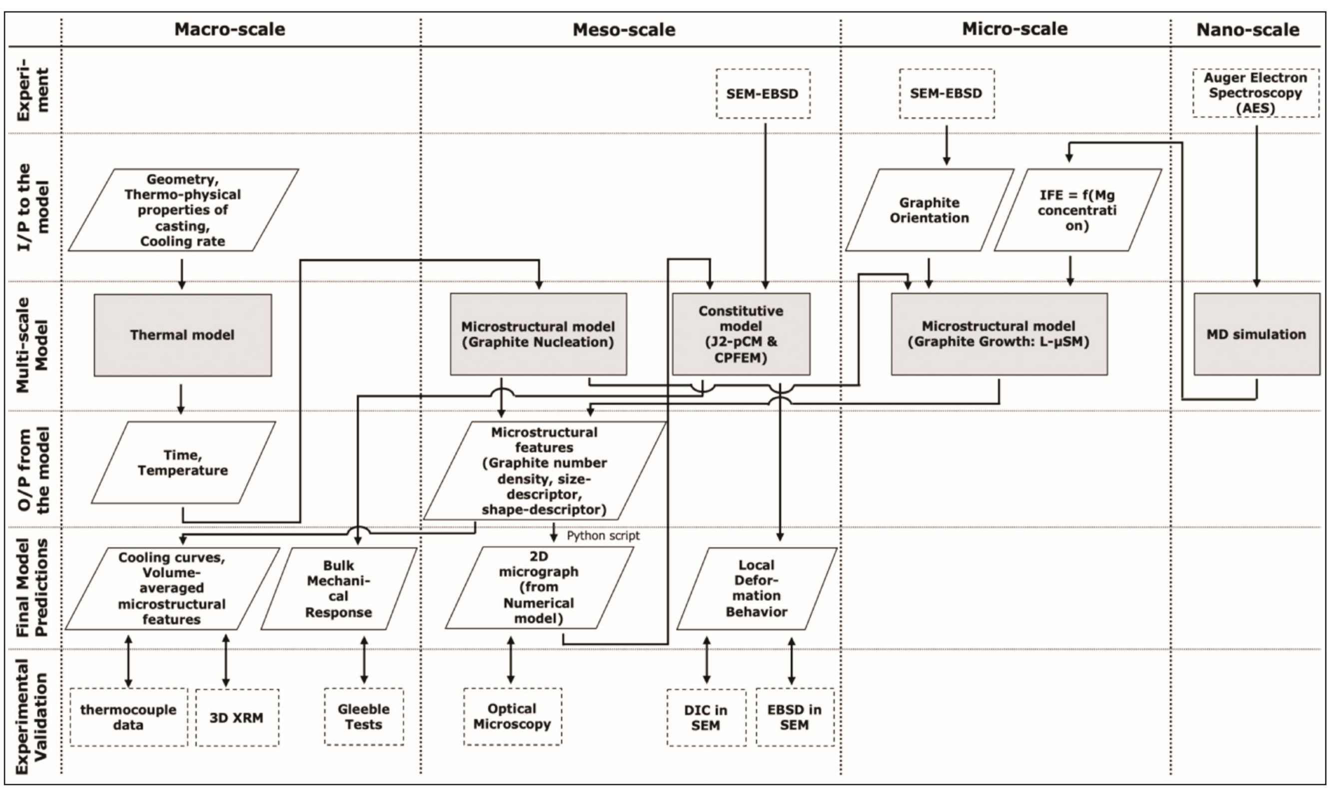


Fig. 2 : Multi-scale modelling and experimental approach for cast irons.

3. Results and Discussion

The final predictions from the multi-scale modelling approach for different types of cast irons were on (1) microstructural features, and (2) microstructure-informed mechanical response. The microstructural features comprise of the following: number density of graphite particles, size of graphite particles (size-descriptors were: thickness, surface area and volume of flake graphite morphology; volume or equivalent radius for intermediate graphite morphology; and radius for spheroidal graphite morphology), shape of graphite particles (shape-descriptors were: circularity or sphericity of intermediate graphite morphology), and volume fraction of phases. The model also predicted cooling curves during the solidification process. The predictions from the microstructure-informed constitutive models were on bulk mechanical response and local deformation behaviour of different types of cast iron owing to their different graphite morphologies. In the bulk mechanical response, the stress-strain curve was predicted. Predictions from the local deformation behaviour were on stress and strain profile at the grain level and on the orientation of grains (that is, texture evolution).

In this article, we will only show a few key results. For a complete set of results, readers can refer to [2,4,7]. Fig. 3 shows the predicted two-dimensional micrographs from the microstructural model for three types of cast iron (GCI, CGI, and SGI). The figure also compares their respective optical micrographs obtained from optical microscopy experiments. From the figure, it is evident that the multi-scale microstructural model was able to capture the size and shape of different morphologies of graphite (flake, intermediate, and spheroidal) in cast iron.

Fig. 4 shows the predictions from the CPFE constitutive model. In Fig. 4a, comparisons were made between the predicted and experimentally obtained bulk mechanical response (engineering stress-strain) of GCI and SGI; while Fig. 4b shows their local deformation behaviour. The yield strength of GCI is ~180 MPa and that of SGI is ~450 MPa (see Fig. 4a). The top row in Fig. 4b shows the synthetic microstructure of an RVE of GCI and SGI generated using DREAM3D software [8]; while its bottom row shows its von Mises stress profile when the RVE was strained to ~0.1% of its gauge length (that is, 50% of offset yield) (marked as a cross in Fig. 4a). Regions whose stresses were greater than the yield strength (~180 MPa for GCI and ~450 MPa for SGI) has been contoured red. This signifies that the local (red) regions have undergone plastic deformation much before the gross yielding took place. The local plastic deformation is highly dependent on graphite morphology and orientation of grains (texture).

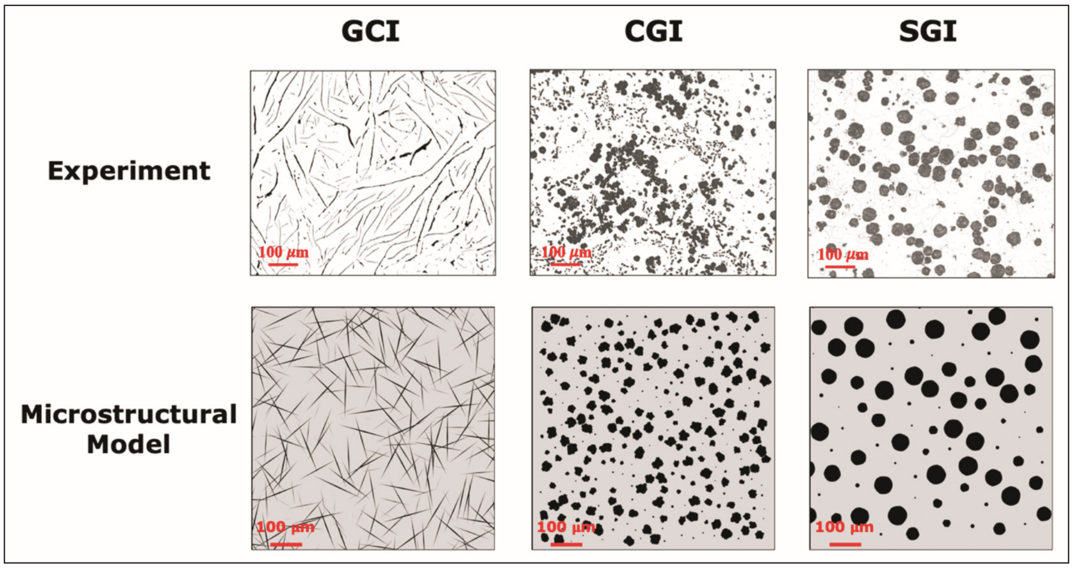
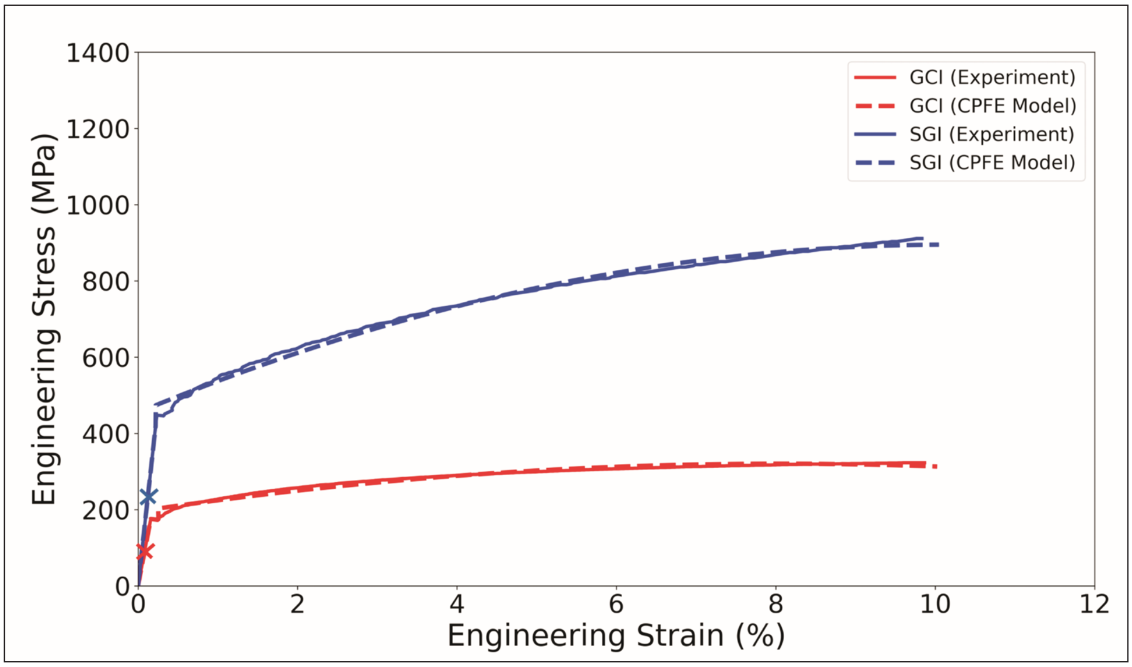


Fig. 3 : Two-dimensional micrographs of grey cast iron (GCI), compacted graphite cast iron (CGI), and spheroidal graphite cast iron (SGI). Micrographs from the top row are obtained from optical microscopy experiments. Micrographs from the bottom row are predicted from a microstructural numerical model.



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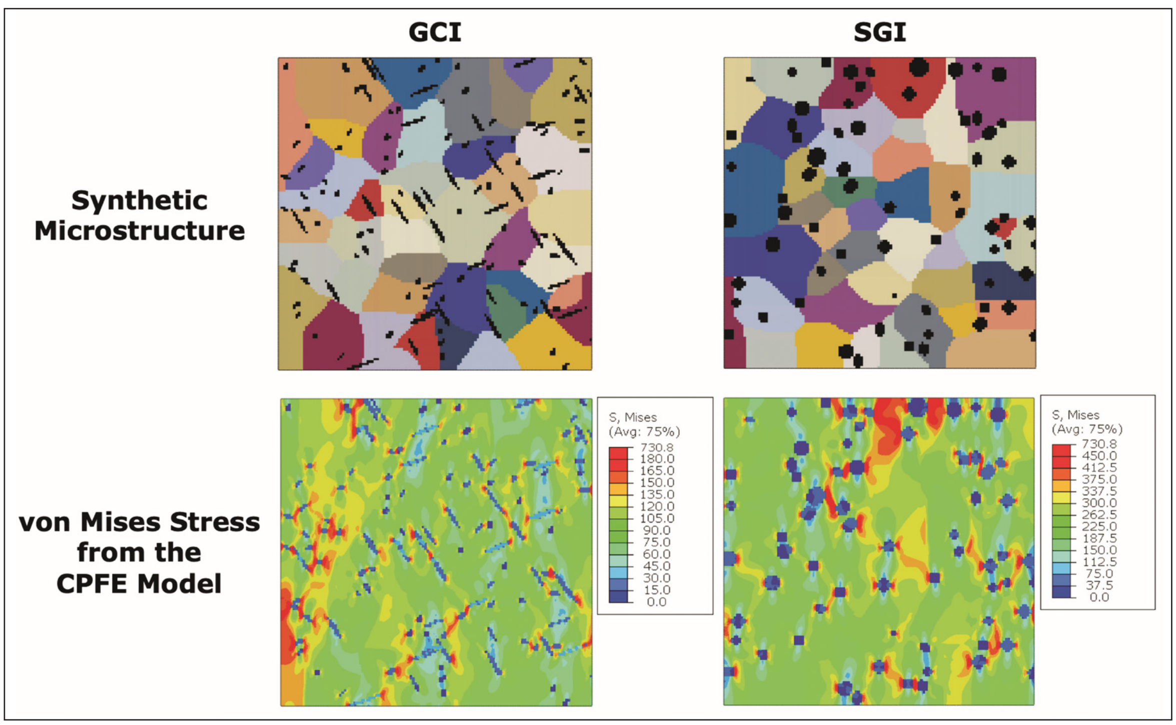

(b)

Fig. 4 : (a) Comparisons were made between experimentally obtained and predicted bulk mechanical response (engineering stress-strain) of grey cast iron (GCI) and spheroidal graphite cast iron (SGI). Experimental data were obtained from Gleeble compression tests. While the crystal plasticity finite element (CPFE) model was used for the predictions. (b) Synthetic microstructure of GCI and SGI obtained from the DREAM3D® software [8]. CPFE predictions of the von Mises stress profile are shown for the same representative volume element (RVE).

4. Industrial Implementation and Implications

Off-highway vehicles use a significant number of castings in their products. For example, a tractor uses ~40% castings by mass. Mass and cost reduction of casting parts using design optimization is a regular practice in these industries. In this section, the practical industrial implementation strategy of the framework has been discussed.

A tractor front axle support (FAS) component, made of GCI or SGI is being considered as a use case. The function of FAS is to (1) support the engine and axle, and (2) carry the loads coming out as a reaction force from the ground. Therefore, the design is very important considering the complex functional requirements. Casting is a preferred choice for manufacturing of this component [9] as the it provides a flexible shape. However, flexibility comes with a significant challenge, that is, certain locations of the casting are critical such as bolt location, sudden change in the section thickness from thin to thick section, and highly stressed location because of external loading (see Fig. 5). In practice, often these locations limit the design flexibility and traditional component engineering approach provides limited scope. In this situation, the multi-scale modelling approach, discussed in this article, will help significantly in producing robust and optimized casting components.

After the component design, a process simulation is carried out to assess the process feasibility (mould filling, flow turbulence, defect). The tool also calculates time-temperature during solidification at selected locations of interest in the component (for example, bolt location, transition from the thin to the thick section, highly stressed region). The multi-scale microstructural model takes time and temperature as input and uses the kinetics of nucleation and growth to predict the microstructural features. The microstructural information served as an input for the J2-pCM and CPFEM constitutive models to obtain the bulk mechanical response and local deformation behaviour. Thus, the estimation of the local deformation behaviour at critical locations of the component due to design features is critical for design decisions. Now, with the availability of such local information around critical features, the product engineer can compare the local stress with material bulk strength and decide rather than assuming uniform bulk material behaviour throughout the component.

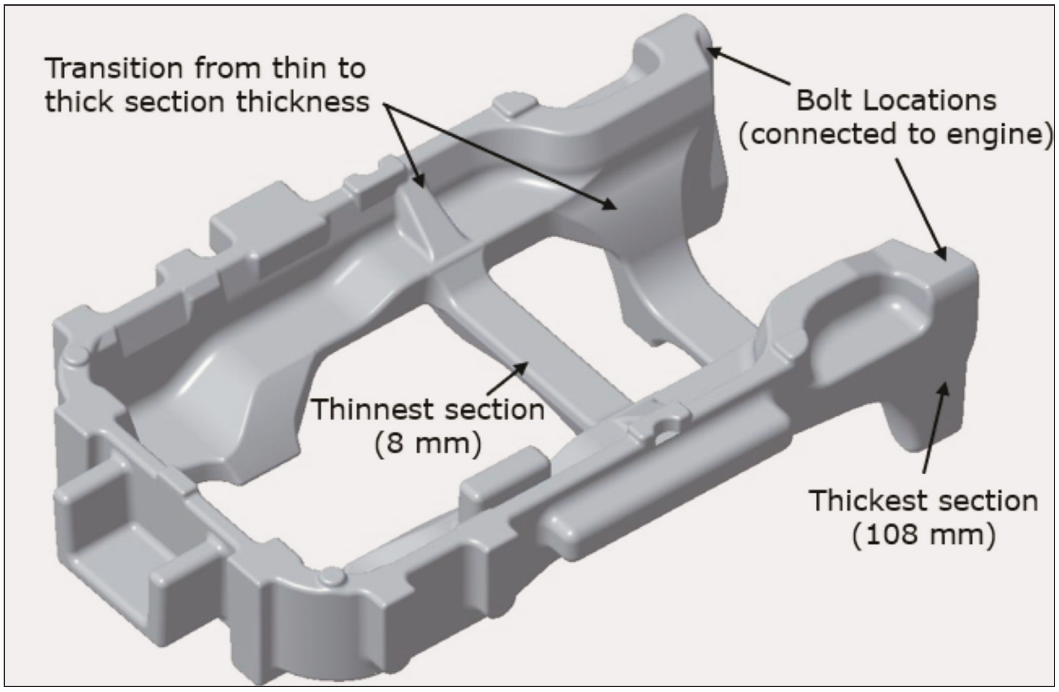

Fig. 5 : Front axle support (FAS). Critical locations are marked. These are: thinnest section (8mm), thickest section (108 mm), transition from thin to thick section, and bolt locations.

5. Summary and Challenges

In this study, the traditional engineering component development workflow was modified by adding a multi-scale (macro, meso, micro, and nano) microstructure and microstructure-informed constitutive models for the casting of different types of cast irons. Experiments were also carried out at various length-scale, which served two purposes: (1) to obtain input parameters to the multi-scale models, and (2) to validate the models' prediction.

At the macro-scale, a thermal model was developed based on the casting geometry, thermo-physical properties of castings, and cooling rate. At the meso- and micro-scale, a microstructural model was developed to predict the microstructural features of cast irons based on the information obtained from the higher length scale (that is, macro-scale). Certain model parameters were also obtained from a much lower length scale (that is, nano-scale). Constitutive models were developed based on the microstructural features to predict bulk mechanical response and local deformation behaviour.

An industrial implementation strategy for the modified workflow was discussed for an actual tractor casting component for design optimization. However, there are intrinsic challenges of a using such higher fidelity approach in industries: (1) computational time to perform simulation of a component (large geometry), and (2) expertise required to handle such a complex framework and to have subject matter knowledge. However, with the advent of quantum computers, it is hoped that performing higher fidelity simulation at a component level will be possible in the near future. Also, simplified tools and software can be developed out of this knowledge which an engineer can easily use without much expertise requirements.

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Technical Article

Accelerating Next Generation Materials Development and Deployment with ICME and Digital Enablement

Gerald Tennyson, Amit Salvi, B P Gautham

Abstract

The framework and methodologies for Integrated computational materials engineering (ICME) have been researched for the last two decades. The ICME has been envisaged to transform the materials engineering and associated decision making with significant industrial applications in materials and component design decisions as well as manufacturing process optimization for accelerated product development. However, the industrial scale-out of this method necessitates a platform approach. In this article, the TCS-PREMAP digital platform for ICME has been presented. The ability to perform multi-scale modelling leveraging ICME approach will be detailed. Furthermore, specific use cases on alloy design for new steel grades and process design with integration of multiple models for hot rolled microalloyed steels will be described. The ability of such platforms to ease decision making for engineers involved in the design, development and manufacturing of novel materials and products in the industry along with ease of knowledge archival for future discovery will be discussed.

Introduction

Materials play a key role in the advancement of any society. However, the development to deployment cycles for new materials is long drawn. This is due to the excessive reliance on serendipity and human intuition for discovery of new materials and extensive lab-scale experiments for proof of concept. Furthermore, the process of scaling up for production frequently demands extensive trial-and-error in a plant, making it very expensive and time consuming. Further, development of material models and uncertainty bounds of properties required for design add significant qualification testing. Extending beyond production, there is an increasing emphasis on product repair throughout its lifecycle and the promotion of recycling and reuse practices at the end of the product's useful life, highlighting the evolving priorities in materials development. This is depicted in Figure 1. While all these factors require a highly interconnected decision system, the reality often differs, with silos persisting across product design, materials, and manufacturing. All of this adds a significant time and cost, often limiting the progress of materials. Accelerating the materials development life cycle, reducing its cost and breaking down the silos in the process requires adopting digital platforms, integrated computational tools, leveraging AI/ML, cross-functional collaboration and promoting knowledge sharing as shown in Figure 2. The concept of Integrated Computational Materials Engineering introduced in [1] is a powerful paradigm that envisaged many of these aspects and transform materials engineering with an aim *to enable the optimization of materials, manufacturing processes, and component design, long before components are fabricated, by integrating the computational processes involved into a holistic system*.

While this holds true on a global scale, India is currently at crossroads, poised with immense potential to transition into a technologically advanced nation and a prominent global manufacturing hub. Despite India's rich history with the then advanced materials, the development of new materials with widespread deployment has been limited in recent times. Leveraging India's substantial digital capabilities, the integration of computational science, AI/ML, and other digital technologies holds the potential to propel forward in this critical domain, enabling significant contributions not only to our nation but also to the broader global community.

TCS Research, Pune

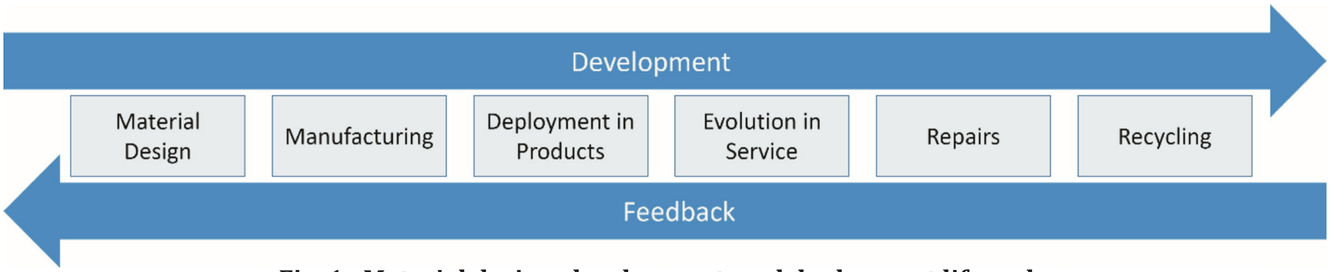

Fig. 1 : Material design, development, and deployment life cycle

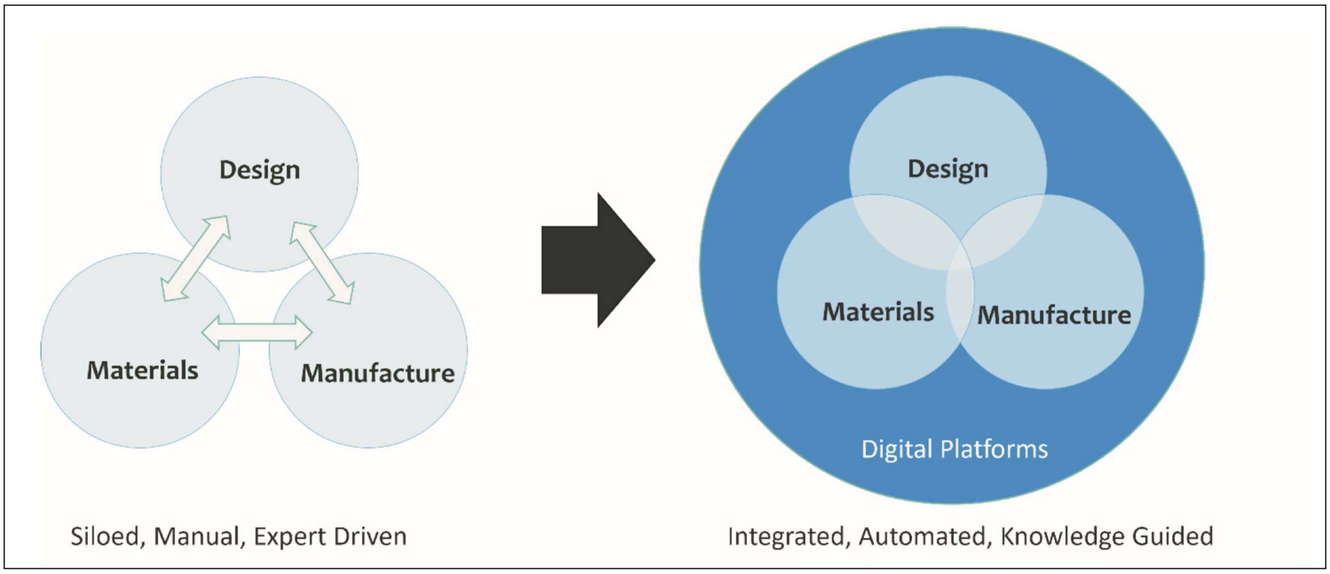

Fig. 2 : Existing Siloed approach vs Digital Enablement with ICME

Materials Development Life Cycle and its Acceleration

Materials for engineering applications are developed for accomplishing a set of target properties and product-performance characteristics. Depending on the specific need and value to be delivered along with cost and other constraints, materials are developed for a set of requirements for either a single product or a class of end-use applications. We present a typical example of the material development life cycle below.

Figure 3 depicts a part of the development life cycle from material design to industrial scale production with an example of development of a new grade of steel sheet for automotive applications. The starting point is to capture a set of requirements such as strength, ductility, weldability, manufacturability etc. based on the market needs for target end-use applications. The ranges for composition and processing conditions are determined by experts with deep knowledge and experience. Subsequently, laboratory scale experimentation is carried out where alloy of a specific composition is produced in few grams to kilograms and processed through relevant thermomechanical treatments and tested for the properties in lab scale equipment, such as Gleeble. Once laboratory-scale testing establishes the alloy chemistry and initial manufacturing process steps, the focus shifts to industrial-scale production. Typical industrial scale production of steel sheets involves over 250 tonnes of steel per heat cast into slabs of cross section in the range of 2000mm x 250mm. These slabs are further processed into sheets about few millimetres in thickness and kilometres in length in rolling mills. The scale up influences the final properties due to aspects such as macrosegregation and microsegregation superimposed on it in casting, microstructural banding in rolling arising due to segregation, etc. Even after trials on the shop floor, it usually takes a few production batches before plant engineers can stabilize the production of a new grade of steel and consistently achieve the desired quality and production conditions at this scale. Finally, the mill product needs to be characterized with its statistical deviation in properties as well as formability diagrams and establish the necessary data for design and deployment in products, which includes further manufacturing steps involving OEMs and their suppliers. Given the emphasis on lightweighting and safety, the entire lifecycle of alloy development to deployment requires a high degree of coordination and collaboration across various stages. However, the sequential nature of these processes often conflicts with the current demand for rapid concept-to-deployment lifecycles. It should also be noted that these experiments and plant trials are time-consuming and incur significant costs, underscoring the need for more agile and concurrent approaches to meet the demands of today's accelerated product development cycles.

All these stages can be significantly accelerated through the computational paradigm of ICME. By leveraging ICME, it becomes possible to significantly reduce the number of trials needed to accomplish the final goal while carrying out some of the key aspects in parallel.

Integrated computational materials engineering (ICME) defined in [1] is a holistic system to enable the optimization of the materials, manufacturing processes, and component design long before components are fabricated, by integrating the computational processes, data and experiments in a systems-engineering framework. This definition is well beyond computational materials science or multiscale modelling and envisages enablement of holistic engineering decisions, often walking backwards from the end goal as shown in Figure 4. It is well acknowledged that an ICME approach can potentially accelerate this process and reduce the time needed from design to deployment of materials in engineered products to 2-5 years. Besides the development of a set of predictive computational materials engineering tools, it was envisaged by the authors of the NRC report that the enabling digital platforms associated with requisite IT infrastructure including collaborative websites, repositories of appropriate data and models will help ICME capabilities and consequently enhance the competitiveness of the industry, in particular, the manufacturing industry. ICME promised to eliminate the growing mismatch between materials and product development cycle.

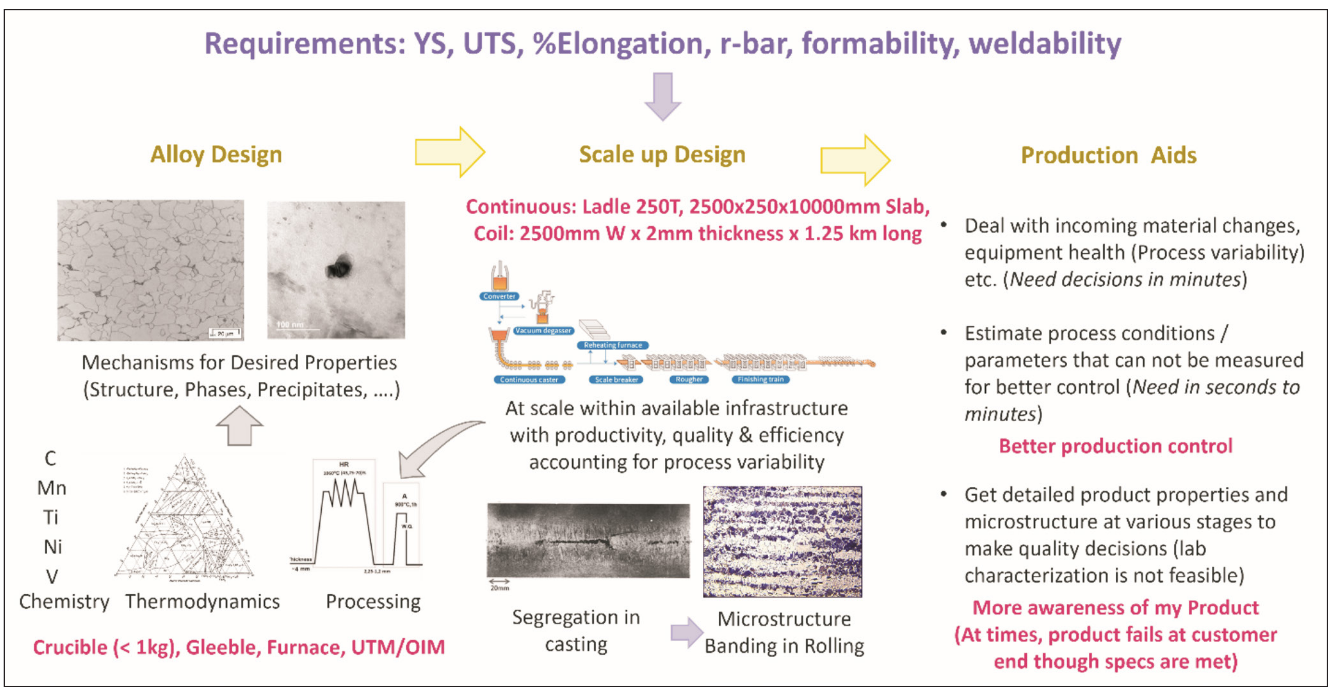

Fig. 3 : Typical Process from Alloy Design, Scale up and Production for New Steel Grades

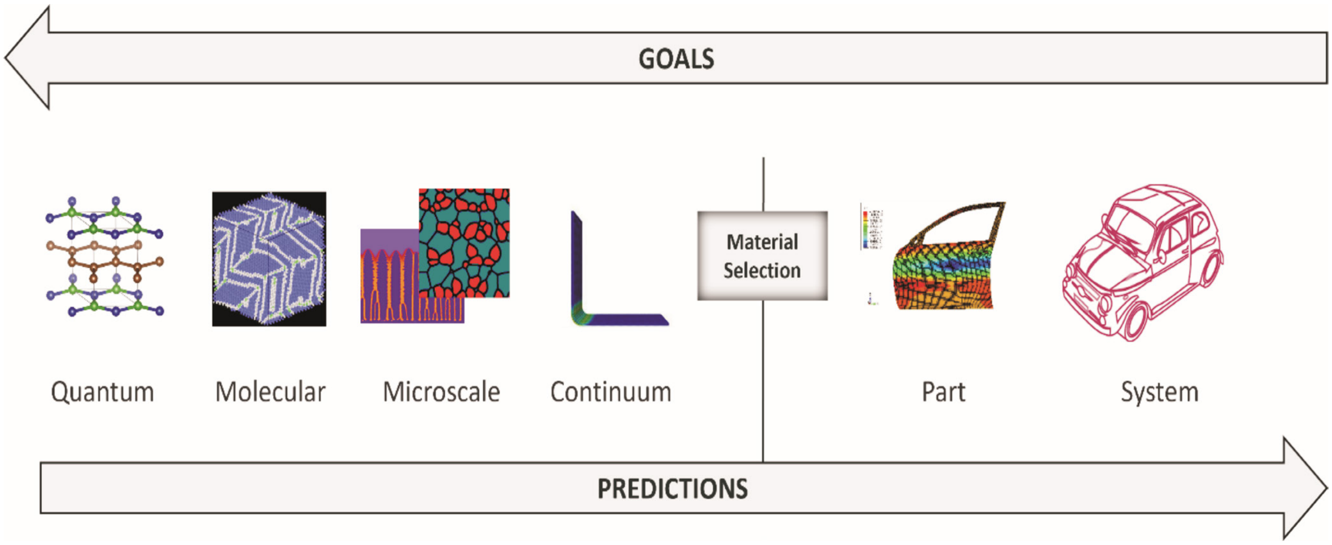

Fig. 4 : Multi-scale modelling leveraging the ICME approach

Extending on this report, TMS conducted a comprehensive study on ICME in 2013 [2] and further elaborated the state of the art with specific focus on key sectors such as automotive, aerospace and maritime industries. This report identified ways to incorporate ICME concepts into the product development life cycle within these industries. Subsequently, TMS released several additional reports aimed to enhance our understanding of the state of the art, gaps and means for industrialization of ICME and allied subjects. These reports include gaps in multi-scale modelling in 2015 [3], the needs and methods for establishing data infrastructure in 2017 [4], validation and verification of computational tools in 2019 [5] and use of Artificial intelligence in 2022 [6].

The practical benefits of ICME have been repeatedly demonstrated across various industries. For instance, Boeing employed early forms of ICME to accelerate the incorporation of composite materials into their aircraft [7]. General Electric (GE) utilized ICME to expedite the adoption of new materials and processes for their gas turbine engines [8]. In the automotive sector, Ford showcased the application of ICME in the development of a new aluminium alloy and casting process for engine blocks. Importantly, these applications not only proved the feasibility of alloy development in-silico but also yielded substantial returns on investment (RoI), with reported RoI exceeding 9. In more recent times, Tesla, the electric vehicle manufacturer, adopted ICME principles to create a novel aluminum alloy and die-casting process. This innovation enabled the production of a single-piece underbody for electric vehicles, resulting in a significant reduction of component footfall by more than 70 individual parts [9].

Research to Realization at TCS

We, at TCS, focus on gainfully leveraging ICME and other computational paradigms along with recent advances in digital technologies in solving challenging materials development related problems for our industry. We have also developed a digital platform TCS PREMAP (Platform for Realization of Engineered Materials and Products) to enable industrial realization of ICME [10]. The practical application of the ICME principles is demonstrated through a case study focused on the design and development of new grades of steel coils. This has been implemented using TCS PREMAP to showcase the effectiveness and capabilities of digital platforms in this context.

TCS PREMAP – Platform for Realisation of Engineered Materials and Products

TCS PREMAP is based on a state-of-the-art, model-driven software engineering paradigm to address the needs mentioned earlier. This platform enables ontological definitions of various entities of interest such as a material, process, equipment, simulation model etc. using metamodels acting as templates [10]. These models are used to express data and knowledge semantically. Various forms of knowledge –e.g. a model with its applicability conditions, a right phase diagram applicable under specific conditions, a thumb rule to set the furnace temperature for curing – can be captured systematically using the ontology built into the platform. This enables easy storage and recall of the relevant information as and when needed, appropriate for the context and intent of the user of that information [11]. This knowledge, in executable or referential form is delivered to users as they undertake execution of workflows for decision making. The platform is designed to be user-friendly, enabling engineers with digital proficiency to use it with ease, requiring little to no coding, particularly for basic tasks such as small computations.

Case study: Integrated computational framework for the design of high strength low alloy (HSLA) steels

HSLA steels are a broad class of steels that achieve higher strength with a much lower alloy content and controlled thermo-mechanical processing. The strength of HSLA steels, also referred as microalloyed steels, is primarily achieved by micro-alloying elements contributing to fine carbide precipitation, substitutional and interstitial strengthening, and grain-size refinement influenced largely by the thermo-mechanical processing conditions. For example, yield strengths surpassing 800MPa can be achieved by microalloying and controlled thermo-mechanical processing as opposed to C-Mn steels with alloying additions such as Ni, Cr or Mo comes to about only 200-250MPa. Designing a HSLA steel for higher strength and formability requires a better understanding of the chemistry and thermomechanical processing conditions, that generally involves a large number of trials and expert knowledge. The processing route includes reheating a cast slab of thickness ~60-200mm to a higher temperature, usually 0.8 TM (~1100-1300^{0}C) and reduced to a strip of thickness ~8-20mm depending on the final requirements, in a hot rolling mill. The reduction usually happens in stages or passes typically ~5-7 passes post which the hot strips are further cooled down in a run-out table (ROT) and coiled. The different process set points across the processes viz., reheating – hot rolling – ROT – coiling are determined by the microstructural changes happening inside the slab/strip. Integrated computational models capturing various phenomena occurring across processes and length scales in the hot strip mill are required to engineer the final microstructure.

An ICME framework to capture the various phenomena in a hot strip mill is developed as shown in Figure 5. The framework captures the microstructure evolution across the process chain (Reheating - Hot Rolling – ROT – Coiling) and predicts the mechanical properties based on the final microstructure. Following approaches have been used to capture various phenomena across the hot strip mill.

1. A phenomenological model is used to predict austenite grain growth during reheating based on the soaking temperature, time and initial precipitate statistics.
2. A mixed analytical numerical approach has been employed to capture the evolution of macroscale thermo-mechanical variables such as strain, strain rate, temperature across the slab thickness and across the passes during hot rolling.
3. CALPHAD approaches are used to predict the strain induced precipitation during thermos-mechanical processing as well as during coil cooling.
4. Recrystallization of austenite during rolling accompanied with precipitation is simulated using a Cellular Automata (CA) model and austenite to ferrite phase transformation in run out table is modelled using phase-field approach.
5. Final mechanical properties of the microstructure obtained are predicted using a FEM based micro-mechanics approach that captures the effect of morphology, grain size distribution, precipitate statistics and phase fractions of the microstructure.

These are illustrated in Figure 5.

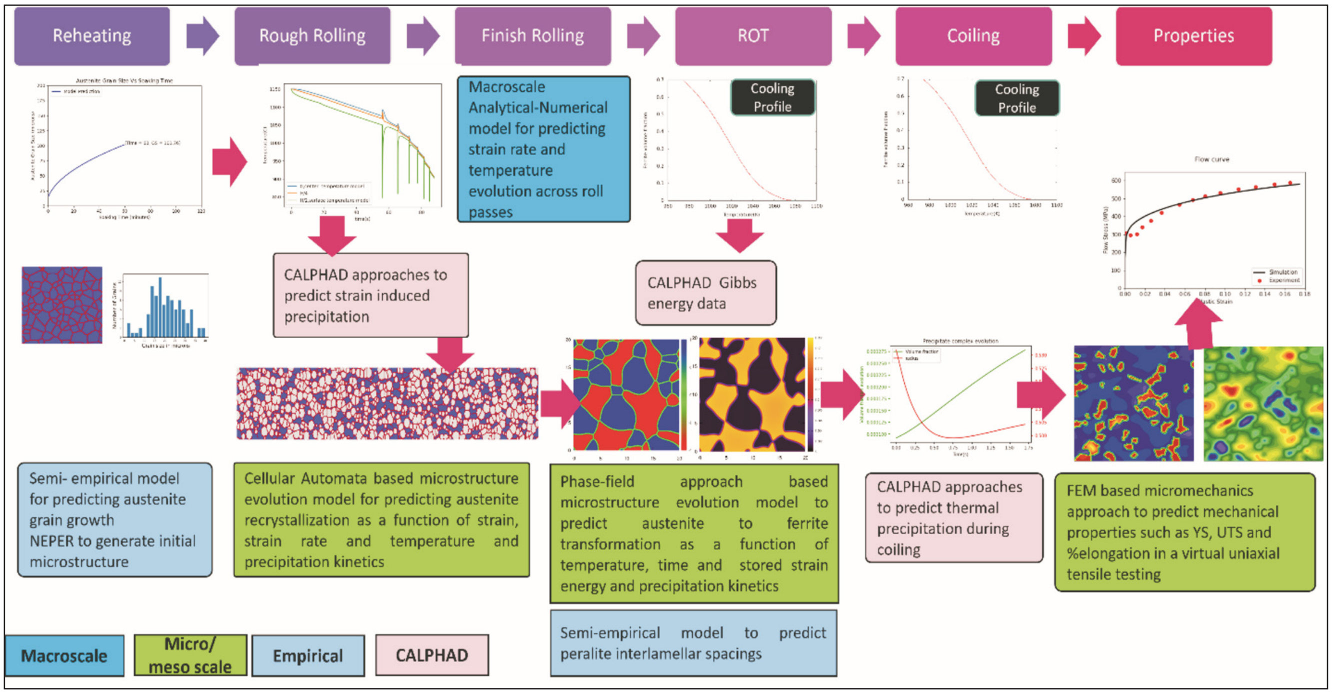

Fig. 5 : ICME framework for alloy and process design showcasing the integration of multiple models across different length scales for design of hot rolled microalloyed steels

Finally, as all these tools are computationally expensive and we need to address inverse problems, a Bayesian global optimization (BGO) approach, an AI based optimization method, is used to minimize the number of iterations involved to arrive at a combination of process parameters from reheating to coiling to achieve the desired mechanical properties. To illustrate the efficacy of this method, we were able to scan a large parameter space and obtain a pareto of feasible conditions in less than 80 simulations as shown in Figure 6.

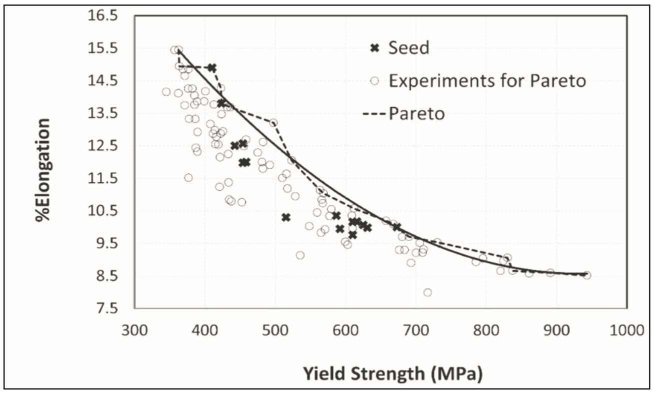

Fig. 6 : Pareto front obtained through Bayesian Exploration

The simulation models described above pertain to multiple processing steps and multiple scales at some key steps. These models are required to be integrated and further constructed in an optimization/ exploration framework. This is achieved using the TCS PREMAP platform and made available to a wide variety of stakeholders who are not well versed in computational tools but need to take the relevant decisions. A workflow for the computation is shown in Figure 7 which leverages past development information, scientific and engineering knowledge and computational tools. Many parameters that are representative of the plant such their capacities, heat transfer coefficients of specific systems needed in simulation, etc., are embedded as elements of knowledge which can also be dynamically updated based on plant performance. Furthermore, the elements of knowledge guide users in making informed decisions when desired outcomes are not achieved. This process is expected to accelerate the alloy development and scaling process significantly and reduce the number of plant trials by at least 50%.

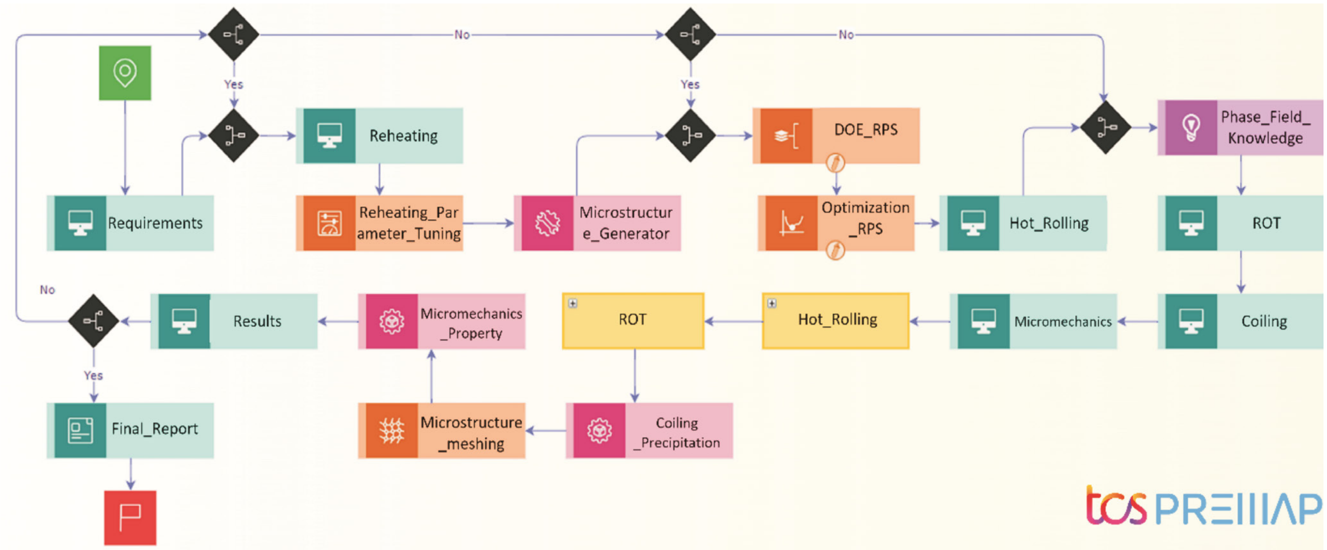

Fig. 7 : Workflow for design of HSLA steels on TCS PREMAP that shows the integration of multiple computational tools, optimization modules and knowledge elements to facilitate easy decision-making

Summary

In this article, we have tried to illustrate means of leveraging computational tools, AI/ML and digital platforms in an ICME paradigm to accelerate materials design and scale up of processes. This can easily be extended further for downstream steps of end product development along with its manufacture.

Digital platforms for ICME, for example TCS PREMAP, as mentioned in this article, are needed to ease decision making for engineers who are involved in the design, development and manufacturing of novel materials and products in the industry. A platform of this kind not only assists in solving immediate challenges but also captures the entire process of discovery and efforts to arrive at the best/ robust solution under various constraints and contexts. As data is generated and decisions get made using the platform, the platform also facilitates the storage of this knowledge for future utilization. Essentially, these curated past data can be used to enhance and enrich the knowledge base for solving a similar problem in the future, thereby also providing a repository of knowledge - addressing another key problem of practical importance in the industry.

A broader paradigm of this nature along with collaborative data and knowledge sharing across all the stake holders can help in accelerating the time needed, reducing the cost and making better materials and material informed products of future.

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परमाणु रिएक्टर Nuclear Reactors
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अनुप्रयोग
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Chapter Activities: Jamshedpur, Kalpakkam, Student affiliate Chapter @ NIT Durgapur

Jamshedpur Chapter

1) The Indian Institute of Metals Jamshedpur Chapter organised a felicitation program for all the IIM ATM and NMA 2022 awardees who are associated with this Chapter on August 8, 2023 at CFE Auditorium, Jamshedpur. Dr. Ashok Kumar, Professor, MME Department, NIT Jamshedpur and Chairperson, IIM Jamshedpur Chapter delivered the welcome address. This was followed by the felicitation of the awardees. Dr. Soumitra Tarafder, Former Adviser Management and Chief Scientist, CSIR-NML graced the occasion as the Guest of Honour. He delivered a short speech and reminiscence the immense contribution of Mr. M S Khan to the progress of the IIM Jamshedpur chapter as an Hon. Secretary. A memento was presented to Dr. Tarafder as a mark of gratitude for honouring the occasion with his presence.

The M.S. Khan Memorial Lecture in the memory of late Mr. M.S. Khan, who had contributed immensely to the progress of the IIM Jamshedpur chapter as an Hon. Secretary was also organized. Shri Ujjal Chakraborti, Managing Director, JCAPCPL & Chairman, CII Jharkhand State Council, has delivered the prestigious M.S. Khan Memorial Lecture on the same day immediately after the felicitation programme on the topic "The Steel; Material of choice- Past, Present, Future". In his lecture he emphasised about global steel production, per capita steel consumption, strategies for increasing steel usages, use of steel as art of beauty, disruption in steel technology and new frontiers of steel usage. He concluded his talk by stating, "Steel is a metal marvel and touches every moment of our lives".

At the end of the talk, a brief question and answer session received good response from the audience. The emcee Ms. Y. Usha thanked the Chief Guest for his talk and requested Dr. A. N. Bhagat, Immediate past Chairperson of IIM Jamshedpur Chapter to handed over a memento to him.

More than 50 people attended the lecture. The program was concluded with a vote of thanks by Dr. Gopi Kishor Mandal, Secretary of IIM, Jamshedpur Chapter.

2) The Indian Institute of Metals (IIM), Jamshedpur Chapter, organised the 11th "Professor S. N. Sinha Memorial Materials and Metallurgy Quiz-2023 (SNSM3Q-2023) for standard XI and XII students at CSIR-National Metallurgical Laboratory Jamshedpur's Auditorium, Burmamines on 11th August 2023. In its 11th successive year, a total of 21 participating schools comprising of 82 students, 21 Teachers, many dignitaries from CSIR-NML, Tata Steel and NIT-Jamshedpur attended the function. The Chief Guest, Dr. Sandip Ghosh Chowdhury, Chief Scientist, CSIR-NML, Jamshedpur inaugurated the programme.

The programme started with floral tribute to Late Prof. Sinha by Dr. Sandip Ghosh Chowdhury, Chief Scientist, CSIR-NML, Prof. Ashok Kumar, Chairman IIM Jamshedpur Chapter, Prof. (Mrs). Gayatri Sinha, wife of late Prof. S N Sinha, Dr. Gopi K Mandal, Secretary, IIM, Jamshedpur Chapter and Dr. A.N. Bhagat, Former Chairperson, IIM Jamshedpur Chapter.

The quiz competition consisted of written screening round followed by a final round. Six teams qualified in the screening round out of 25 teams, representing from four schools, namely - Loyola School Jamshedpur, Narbheram Hansraj English School, Vidya Bharati Chinmaya Vidyalaya, DBMS English School and DAV Public School, Jamshedpur. After series of interesting rounds like multiple choice, hint, picture, dumb charades and materials history, Ms. Ankita Dey Laik and Madhav Varshney of Loyola School Jamshedpur were declared champions. Mr. Arunesh Gadia and Priyanshu Chakraborty of DBMS English School, Jamshedpur got Second Rank. The Quiz winners and Runners-up teams were felicitated with Trophies and certificates.

Prof. Ashok Kumar, Chairman, IIM Jamshedpur chapter welcomed the gathering. While delivering the inaugural address, Chief Guest Dr. Sandip Ghosh Chowdhury said," Prof. Sinha had a great role in building the student fraternity in metallurgy as Head of Metallurgy department of NIT Jamshedpur, and Dean / Principal, NIT as well as Director, NIFFT

Ranchi. He was a teacher of eminence and would be remembered by everyone who came in his contact". Dr. Ghosh Chowdhury also added, "Students may consider the materials engineering / metallurgical job seriously which will help the Nation in long run". Prof. Sinha played a significant role while inspiring his student communities".

The entire programme was highly appreciated by the students, participants, staffs and dignitaries from Tata Steel, CSIR-NML and NIT Jamshedpur. Dr. Gopi K Mandal, Secretary proposed the vote of thanks acknowledging the unrelenting support of entire organizing team and enthusiastic participation of school students.

Kalpakkam Chapter

31st Prof. Brahm Prakash Memorial Materials Quiz (BPMMQ 2023)

IIM-Kalpakkam Chapter conducted the 31st Prof. Brahm Prakash Memorial Materials Quiz (BPMMQ) at Indira Gandhi Centre for Atomic Research, Kalpakkam during September 8-9, 2023. A total of thirty nine teams comprising of seventy eight students of class XI and XII accompanied by escorts and office bearers from eighteen chapters across India participated in this flagship programme of IIM.

On September 8th, 2023, the Metal Camp programme commenced with welcome by Dr. V. Karthik, Vice-Chairman, IIM Kalpakkam chapter and special address by Dr. M. Vasudevan, Associate Director, MDTG & Chairman, IIM Kalpakkam Chapter. Video films on "DAE; a glorious past and resplendent future" and "FBTR Breeds Success" highlighting the milestones of DAE and the flagship research reactor at Kalpakkam were screened. This was followed with visit of the participants to the facilities at Kalpakkam namely Fast Breeder Test Reactor (FBTR), Madras Atomic Power Station (MAPS) and the Prototype Fast Breeder Reactor (PFBR).

On September 9th, 2023, the quiz programme commenced with the preliminary rounds held in six parallel sessions. The winner and runner of each session contested in semifinal round held in two parallel sessions. The welcome address for the event was delivered by Dr. Divakar Ramachandran, Director MMG and MSG & Chairman BPMMQ-2023. The souvenir BPMMQ 2023 Digest containing the details of all BPMMQ events held in previous years, essay articles selected for elocution contest and special messages from dignitaries was released on this occasion by Dr. N. Sivaraman, Director, MCMFCG, IGCAR. This was followed by Prof. Brahm Prakash Memorial Lecture 2023, delivered by Prof. B. S. Murty, Director, Indian Institute of Technology, Hyderabad and Vice President, IIM. Prof. Murty enthused the students in the field of Materials Research and instilled in them a passion for lifelong learning through the excerpts from his experiments in research. He encouraged students to have a broad outlook and achieve the goals with hard work and commitment. Prof. Murty proceeded to share with students the various options for higher education in India, and informed the wider educational community about exciting developments in open education and continuous learning.

Shri Avinash Mudaliar, a renowned quiz master from Mumbai conducted the Grand finale of BPMMQ-2023 comprising of total of six teams (three from each semi-final round). The teams included Jamshedpur, Chennai-A, Kalpakkam-C, Varanasi-A, Varanasi-B and Angul-A. The Finale round of the 31st BPMMQ comprised 8 sub-rounds, arranged in a riveting fashion. The teams were allotted their seating positions based on their ability to identify crystal gemstones. The first two rounds were conducted in alternating clockwise and anti-clockwise seating order, with questions ranging from structures inspired by metals, paleometallurgy, appearances of materials in pop-culture, notable scientific achievements in the fields related to materials, etc. This was followed by a buzzer round, which tested the ability of students to think on their feet and arrive at accurate answers despite facing time pressure. The buzzer round was followed by grid-rounds, where each contesting team got the opportunity to pick a theme of their choice. Grid rounds featured themes such as ancient metallurgy, materials in food, elements and isotopes, nuclear scientists, materials in construction, etc. The winner of BPMMQ 2023 was Chennai Team–A comprising of Mr. R. Shyam Sundar and Mr. Arjun Ananthakrishnan of PSBB Senior Secondary School, Chennai. Angul-A comprising of Mr. Nissim Sahoo and Mr. Yash Pratap Singh of Delhi Public School, Angul won the second place.

The essay cum elocution contest for the quiz participants also was well received this year. The essays were invited from students on the topics, (i) Materials for carbon capture technology (ii) Role of Artificial intelligence (AI) and Machine Learning (ML) in advancement of materials research and (iii) Hydrogen storage and its use in transportation. A total of twenty eight essays were received and eight best essays were selected for elocution contest. The selected participants rendered excellent and flawless elocution and was judged by a three member jury of eminent experts from IGCAR, Kalpakkam. Mr. Aritro Shome of MP Birla Foundation HS School, Kolkata was the winner of Essay/Elocution contest and the two runners up positions were awarded to Ms. Ankita Dey Laik of Loyala School Jamshedpur and Ms. Tanisha Jena, DAV public School, Dera, Angul.

The Winner and Runner teams of the Quiz and the elocution contest were awarded with prizes by chief guest Prof. B. S. Murty. The event was successfully conducted with generous financial support from several well-wishers and promoters of science, including The IIM, Kolkata; IGCAR, Kalpakkam; Department of Atomic Energy, JSW Centre, Mumbai; DRDO, New Delhi; Tata steel, Jamshedpur, Hindalco Industries; NFC, Hyderabad; MIDHANI, Hyderabad; NPCIL, Mumbai; MAPS, Kalpakkam; HWB, Mumbai and several leading firms dealing with metallurgical equipment and services. Dr. Diptimayee Samantaray, Convener, BPMMQ-2023 proposed a vote of thanks and coordinated the event along with Dr. Sainath, Co-Convener, BPMMQ-2023.

Prof. B.S. Murty delivering BPMMQ-2023 Lecture

Release of BPMMQ-2023 Digest

Shri. Avinash Mudaliar, the Quiz Master, conducting BPMMQ-2023 Grand Finale

Prof. B.S. Murty, Dr. R. Divakar and Dr. M. Vasudevan distributing the prizes to winners of Essay/Elocution contest and Quiz of BPMMQ-2023

Student affiliate Chapter @ NIT Durgapur

In the evening of 19th Sept 2023, IIM Durgapur Student affiliate Chapter organised its 4th Foundation Day celebration at NIT Durgapur in the Golden Jubilee Auditorium of Metallurgical and Material Engineering(MME) Dept. The programme went live with wide participation from faculty, students, student members, life members and industry experts including senior officials from DSP(SAIL) and made it a perfect industry-academia symbiotic collaboration. The programme was started with lamp lighting ceremony by Shri Lohitendu Badu, Secretary IIM Durgapur Chapter & GM, DSP-SAIL, Durgapur, and Professor Bera, HoD, MME and Dean of NIT Durgapur. Four years back, exactly on that date the student chapter was established here with the parental support and guidance by the IIM Durgapur Chapter. The Secretary, IIM Durgapur Chapter, in his inaugural address asked students and faculty to increase the participation in form of activities and by enhancing the student membership strength for which all support shall be provided by the parent chapter IIM Durgapur Chapter. HoD and Dean advised students to organise more such technical programme. To make the occasion memorable, a cake cutting ceremony was organised, followed by two technical talks. The first talk was on “Super capacitors” which was delivered by two students namely Shri Badal Singh and Shri Baivav Das. The second talk was on “Study of Dislocations under applied stresses using Dark field X ray microscope” delivered by Ms. Dayeeta Pal, Researcher and PhD student from Stanford University, USA.

Both the lectures were on contemporary topics and evoked active brain storming and discussions from audience during question hours. Faculty coordinator Dr. A Mondal and Student coordinator Shri Rohan Pal gave vote of thanks at the end of the event.

Shri Lohitendu Badu @lamp lighting ceremony

@ the event at NIT Durgapur

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News Updates Domestic

Availability of green hydrogen to reduce dependence on coal in steel making: Tata Steel CEO

The availability of green hydrogen as a fuel will help reduce India's dependence on coal for steel making, Tata Steel CEO and MD TV Narendran said. Narendran made the remark at the National Management Convention session of All India Management Association (AIMA) here.

"The way steel is made is changing and will continue to change further, as the industry is putting up new plants... Availability of hydrogen as a fuel and reductive is the key to reducing dependence on coal," he said, adding that scrap will replace ore as the main input.

In January 2023, the Union Cabinet approved the National Green Hydrogen Mission with an outlay of Rs. 19,744 crore with an aim to make India a global hub for manufacturing this clean source of energy.

Tata Steel plans to scale up the usage of hydrogen in the steel-making process after the successful completion of the pilot project at its Jamshedpur plant in Jharkhand, Narendran told PTI recently.

https://energy.economictimes.indiatimes.com/ (27.9.23)

Scindia discusses ways to incentivise green steel production with various stakeholders

Union Steel Minister Jyotiraditya M Scindia held a meeting with five task forces and discussed a range of issues, including incentivising green steel production and financing options for decarbonising the industry. Key stakeholders, industry experts, and government officials attended the meeting to discuss ways to achieve sustainability and decarbonisation in steel production, the Ministry of Steel said in a statement. The meeting was also attended by Steel Secretary Nagendra Nath Sinha, chairpersons of the five task forces and other senior officials.

"Held a fruitful discussion with 5 of our 13 task forces. Defined a roadmap to tackle inevitable challenges through a multi-pronged approach, including renewable energy uptake, skill development, incentives, and potential pathways for decarbonisation," the minister said.

The task force on finance, led by Sunil Mehta, the Chief Executive of Indian Banks' Association, provided valuable insights into financing options for decarbonising the Indian steel industry, the ministry said.

The Economic Times (29.9.23)

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Achievements Dr S K Jha

Dr. S K Jha, CMD, MIDHANI has been conferred with an Excellence Award on the occasion of Engineers Day on 15.09.2023 jointly organised by Lions International Dist 320-B & Leaf Association. Dr. Jha, a Life Member of IIM, was felicitated with an excellence award for his dedicated contribution towards the metallurgy field and Atmanirbhar Bharat by the chief guest of the event Resu Malla Reddy, pmjf, District Governor of Lions International.

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Crude Steel Production July 2023 (World)

Crude Steel production by region

	Jul 2023 (Mt)	% change Jul 23/22	Jan-Jul 2023 (Mt)	% change Jan-Jul 23/22
Africa	1.4	26.1	9.0	7.0
Asia and Oceania	119.9	9.1	828.4	1.7
EU (27)	10.3	-7.1	76.7	-10.3
Europe, Other	3.6	5.1	23.8	-11.7
Middle East	3.1	-3.9	26.2	2.3
North America	9.4	-1.2	64.1	-3.5
Russia & other CIS + Ukraine	7.4	9.3	51.2	-0.8
South America	3.4	-8.4	23.7	-7.4
Total 63 countries	**158.5**	**6.6**	**1,103.2**	**-0.1**

The 63 countries included in this table accounted for approximately 97% of total world crude steel production in 2022. Regions and countries covered by the table:

- **Africa:** Egypt, Libya, South Africa, Tunisia
- **Asia and Oceania:** Australia, China, India, Japan, Mongolia, New Zealand, Pakistan, South Korea, Taiwan (China), Thailand, Viet Nam
- **European Union (27)**
- **Europe, Other:** Macedonia, Norway, Serbia, Türkiye, United Kingdom
- **Middle East:** Iran, Qatar, Saudi Arabia, United Arab Emirates
- **North America:** Canada, Cuba, El Salvador, Guatemala, Mexico, United States
- **Russia & other CIS + Ukraine:** Belarus, Kazakhstan, Russia, Ukraine
- **South America:** Argentina, Brazil, Chile, Colombia, Ecuador, Paraguay, Peru, Uruguay, Venezuela

Top 10 steel-producing countries

	Jul 2023 (Mt)	% change Jul 23/22	Jan-Jul 2023 (Mt)	% change Jan-Jul 23/22
China	90.8	11.5	626.5	2.5
India	11.5	14.3	79.9	9.0
Japan	7.4	0.9	51.2	-3.9
United States	6.9	0.5	46.8	-2.3
Russia	6.3 e	5.8	44.2	2.8
South Korea	5.7	-9.0	39.4	-1.8
Germany	3.0	-0.5	21.5	-4.6
Türkiye	2.9	6.4	18.8	-13.5
Brazil	2.7	-4.7	18.6	-8.6
Iran	2.0	-1.5	18.1	4.1

e - estimated. Ranking of top 10 producing countries is based on year-to-date aggregate

Source : worldsteel.org


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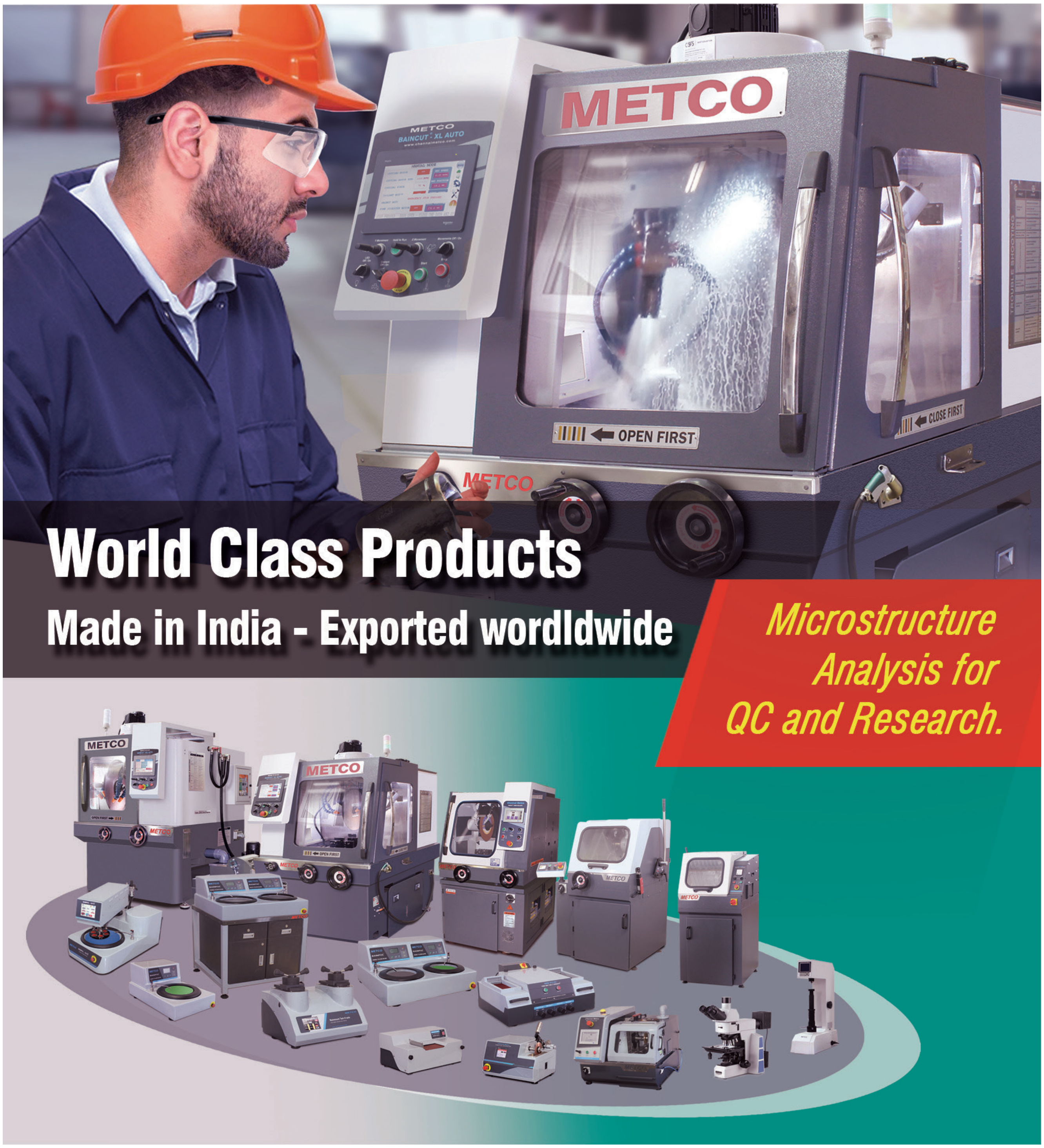
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Non-Ferrous Metals Statistics Domestic Scenario

Production (unit : Lakh Tonnes)

	Aug'23	Jul'23	Jun'23	2022 - 23	2021 - 22
ALUMINIUM					
National Aluminium Co Ltd	0.38	0.37	0.39	4.60	4.60
Hindalco Industries Ltd*	1.13	1.12	1.09	13.22	12.94
Bharat Aluminium Co. Ltd	0.49	0.49	0.48	5.69	5.80
Vedanta Ltd	1.48	1.50	1.43	17.22	16.92
TOTAL	**3.48**	**3.48**	**3.39**	**40.73**	**40.26**
*Renukoot, Hirakund, Mahan, Aditya					
ZINC (One major producer)					
Hindustan Zinc Ltd	**0.63**	**0.58**	**0.69**	**8.21**	**7.76**
COPPER (Cathode)					
Hindustan Copper Ltd	0	0	0	0.000073	0.62
Hindalco (Birla Copper)	0.35	0.31	0.25	4.07	3.59
Vedanta Ltd.	0.12	0.11	0.10	1.48	1.25
TOTAL	**0.47**	**0.42**	**0.35**	**5.55**	**4.85**
LEAD					
Hindustan Zinc Ltd	**0.20**	**0.16**	**0.16**	**2.11**	**1.91**

Source : https://mines.gov.in/

Prices in India (as on 30th September, 2023)

(Mumbai Local Price in Rs. / kg)

Product	Rs. / kg	Product	Rs. / kg
Copper Armature	689	Aluminium Ingot	217
Copper Cathod	741	Aluminium utensil	173
CC Rod	746	Zinc Ingot	233
Copper Cable scrap	711	Lead ingot	189
Brass Sheet Scrap	507	Tin Ingot	2138
Brass Honey Scrap	476	Nickel Cathod	1643

Source : https://mtlexs.com/


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Second Announcement

IIM Metallurgy Materials Engineering

IIM-ATM 2023

77th Annual Technical Meeting of the Indian Institute of Metals

22nd – 24th November 2023

Venue: KIIT, Bhubaneswar

Organisers: IIM Sambalpur Chapter, IIM Angul Chapter, IIM Bhubaneswar Chapter and Hindalco Industries Ltd.

77th ATM 2023, an annual flagship event of IIM will be attended by many prominent industry captains, technical experts, senior academicians and students from various technical institutions from all parts of India and abroad. The ATM's multiple sessions are a centralised hub for sharing knowledge, exchange of ideas and deliberating new initiatives.

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MR SS MOHANTY
MD & CEO,
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CONVENOR

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Advisor,
Hindalco Industries Ltd.

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- **300** Poster Presentations

22nd November
- Inauguration of IIM-ATM 2023
- Inauguration of Technical Exhibition
- International Symposium

23rd November
- Inauguration of 77th ATM Technical Meeting
- IIM Award Ceremony
- IIM Plenary Lectures

24th November
- 8 Parallel Technical Sessions
- Valedictory Session

The IIM-ATM 2023 Organizing Committee, cordially invites you to join for a wonderful learning, sharing and networking experience, in Bhubaneswar - The City of Temples and the emerging Educational and Health Services hub of Eastern India. We look forward to your valuable participation and overwhelming support.