Remarks on Special Issue on Materials Characterization Research and Mathematical and Numerical Analysis

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The integration of observation and analysis technologies for metallurgical microstructures and chemical states (hereafter referred to as analytical technologies) with numerical simulation technologies for material flow, structure, reaction processes and mechanical states (hereafter referred to as computational modeling) has made the development of steel materials more efficient than ever before. Steel material development must be approached from two complementary perspectives: compositional and microstructural design to achieve high performance under service conditions, and microstructural control technologies within the manufacturing process. Analytical technologies and computational modeling serve as the "translational interface" bridging these two perspectives. To meet market demands, deliberate design of microstructures and the processes to control them are indispensable, and this in turn requires continued advancement of the analytical and computational technologies that support these efforts.

Analytical technologies have enabled the observation of fine microstructures and chemical states of materials that were previously difficult to observe, providing essential insights for manufacturing process optimization and design of new materials. Through the use of high-energy beams, three-dimensional structures and chemical states of steel products and their raw materials, such as iron ore and coal, can now be observed. Furthermore, advances in techniques such as electron microscopy and atom probe analysis have enabled atomic-scale structural analysis of steel products. These developments have made it possible to design and precisely control material microstructures at the nanometer and even atomic scale, bringing the development and practical implementation of higher-performance steel materials within reach.

Meanwhile, computational modeling technologies have continued to evolve as foundational tools that theoretically support the understanding of material properties, enabled by the dramatic increase in computational power. In recent years, techniques such as phase-field modelling for microstructure evolution, first-principles calculations and molecular dynamics simulations for analyzing atomic-scale structures and behaviors have increasingly been applied to practical materials, providing new degrees of freedom in steel material design. In addition, the development of continuum models capable of handling complex systems involving gases, liquids, and solid particles has progressed, allowing the simulation of internal states and behaviors in ironmaking processes at a significantly lower cost than before. Furthermore, the appli-

cation of AI technologies, including rapidly advancing machine learning, to materials analysis, materials design and equipment design is also progressing, raising strong expectations for further innovation in materials development.

In this special issue, we present an overview of the analytical and computational modeling technologies possessed by Nippon Steel Corporation and Nippon Steel Technology Co., Ltd., together with representative examples of their applications, in order to explore new possibilities in steel materials development. We hope that this special issue will serve as a starting point for further advances in the field of steel materials research and development.