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## Remarks on Special Issue on Computational Science: Progress of Computational Science and Its Position in the Iron and Steel Industry

*In November 2011, the “K” computer won the Peak Performance Award of Gordon Bell Prizes after registering an effective performance of 3.08 petaflops in the first-principles calculation of the electrical conductivity of a silicon nanowire consisting of 100,000 atoms. Furthermore, in terms of theoretical performance based on the LINPACK benchmark, K topped 10 teraflops, thereby securing its position as the world’s fastest computer for a second consecutive term following its June 2011 high of 8 teraflops. Japan’s “Earth Simulator” was the world’s fastest supercomputer for five consecutive periods (two and a half years) from June 2002. Finally, a Japanese supercomputer has regained the world championship in this particular field. Supercomputers had achieved a double-digit performance improvement over 20 years, from 100 megaflops in the early 1970s to 10 gigaflops in the early 1990s. However, since the early 1990s, improvements in computational performance have been accelerating: current performance has been enhanced a million-fold in two decades, to 10 petaflops in 2011. With these performance improvements in computers and progress in computational science, its application to the iron and steel industry has been expanding, although this is not entirely attributable to the development of supercomputers.*

*Following the structural dynamic analysis based on the finite element method, computational fluid dynamics to solve Navier-Stokes equations have been introduced to the iron and steel industry as a form of computational science with industrial applications. Today, it is used to control and optimize steel-making-process operations. Structural dynamic analysis has long been applied to analyze plastic deformation to enhance the accuracy of forming in the rolling processes and analyze the deformation and strain of slabs to restrain their cracking and macrosegregation in the continuous casting process. Recently, it has also been employed to analyze secondary work processes for steel products. Today, the application of structural dynamic analysis is expanding into the prediction of material properties based on the crystal plasticity finite element method that reflects crystal orientations in the plasticity/rigidity matrix.*

*On the other hand, computational fluid dynamics is utilized to analyze the advection diffusion of refining agents and non-metallic inclusions in the refining vessels and continuous casters. Specifically, it is applied in case studies to secure the reaction time for injected refining agents*

*and promote the floating separation of non-metallic inclusions. From the same standpoint, computational fluid dynamics is also applied in the analysis of the molten steel flow control using electromagnetic force. In addition, it is used in simulations of the refining reactions combining the molten metal flow and slag-metal reaction and in total simulations of the blast furnace reactions combining a flow analysis of the gas phase, liquid phase, solid phase, and powder with various reactions that occur in the blast furnace. In flow analyses, the particle methods, such as DEM and SPH, are also applied to analyze blast furnace reactions, casting, and solidification processes, and cooling water flow, etc. in recent years. Details about the application of computational science to the steel manufacturing processes are to be presented in a separate volume. Herein, the focus is on computational science that helps to develop new steel materials.*

*If the development of new steel materials is equated to navigation at sea, then the phase diagram serves as a chart for navigation. Computational thermodynamics strives to make predictions based on the computations of the phase diagram. Since the early 1970s, the calculation of phase diagrams (CALPHAD) technique, which calculates phase diagrams first by evaluating the free energy of each phase on the basis of empirical data and then repeating the thermodynamic equilibrium calculations using the evaluated free energies, has been developed. The 40th International Conference on CALPHAD was held last year. In Japan as well, the Society for the Joint Study of Alloy Phase Diagrams (Chairman: Jin-ichi Takamura, Vice-chairman: Taiji Nishizawa) was inaugurated in 1986 with the backing of the Japan Institute of Metals and the Iron and Steel Institute of Japan, amongst others. Today, the society works as the No. 172 Committee for Alloy Phase Diagrams of the Japan Society for the Promotion of Science.*

*In the field of computational thermodynamics, not only has the empirical approach been developed to calculate phase diagrams from databases obtained by experiments, but also has a non-empirical technique to predict phase diagrams from thermodynamic properties obtained by first-principles calculations. Thus, there are cases where experimentation and first-principles calculations complement each other. Japanese steelmakers have been active in introducing the new technique. Nippon Steel Corporation, which has been positively utilizing computational thermodynamics, won the first APDIC Industrial Award from the Alloy Phase Diagram International Commission in 2003. JFE, Baosteel, ArcelorMittal, and POSCO also received the same award in subsequent years.*

*Although the equilibrium phase diagram shows the phase fractions and their compositions of a given material in its equilibrium state, actual steel materials are often used in the non-equilibrium state. Therefore, an approach has been developed and used to analyze the phase transformation in a specific material process in terms of the diffusion of solute and local thermodynamic equilibrium at the interface by applying computational thermodynamics. Recently, it has also become popular to predict the phase morphology, using the phase-field (PF) method considering the effect of phase interfacial energy as well. In Japan, the pioneering study in this particular field dates back to the early 1990s. Analyses with the PF method can be carried out using the Monte Carlo (MC) method also. Although the MC method requires a computing load larger than that required by the PF method, it permits the handling of the nucleation process, which cannot be handled by the PF method. Secondary recrystallization can also be analyzed using*

*the vertex method.*

*The Kohn-Sham equation was the primary factor in expanding the application of first-principles calculations. The density functional theory that permits the solving Schrödinger's wave equation paved the way for calculations of the electronic structure and energy of practical materials. Kohn won the 1998 Nobel Prize for chemistry, along with Pople, developer of the quantum chemistry calculation program "Gaussian." This method is also used for the calculation of the total energy of the ordered phase, which contributes in the first-principles calculation of the phase diagrams described above. In the first-principles calculation of phase diagrams, interatomic potentials are obtained from the above total energy by the cluster expansion method and a thermodynamic equilibrium state is repeatedly obtained using either the cluster variational method or MC method with the consideration of the entropy terms. On the other hand, it is also possible to obtain the activity coefficient and interaction parameters on the basis of a total energy calculation for a system including solutes.*

*Next, for the atomic structure analysis, the molecular dynamic method can be cited. It started as a classic molecular dynamic method in which interatomic potentials prepared on the basis of empirical facts are used to obtain the force acting upon the atoms first, and then the Newtonian equation of motion is solved to simulate the motions of atoms. Then, the embedded atom method (EAM) potential that considers multibody effect was developed. The EAM was followed by the epoch-making Car-Parrinello method in 1985. It is the first-principles molecular dynamic method in which the exchange-correlation energy is approximated by the density functional theory, the wave function is renewed each time the atom position changes, and the Hellmann-Feynman force is obtained to simulate the atomic motion. This method has simplified the first-principles calculations of not only disordered phases but also surfaces, interfaces, dislocations, point defects, etc. where the atomic structure is disturbed. At the same time, it has allowed for the first-principles calculations of atomic-level dynamic processes, such as the progress of reactions and fracture cracking, etc.*

*At the computational physics subcommittee meeting of the Computer-Aided Materials and Molecular Design (CAMM) forum, Nippon Steel Corporation participated in the joint development by 14 member companies of a first-principles molecular dynamic universal program based on the Car-Parrinello method. The jointly developed program, CAMP-Atami, was registered with the Japan Chemistry Program Exchange (JCPE) in 1994 and won the JCPE Excellent Program Award for fiscal 2001.*

*For promoting domestic computer software in the field of computational science and enhancing computer performance, national projects have been formulated. Since 2002, first through the "Development of Frontier Simulation Software for Industrial Science" and "Development of Revolutionary Simulation Software" and then through the "Next-Generation Supercomputer Projects: Grand Challenge Next-Generation Integrated Nanoscience and Next-Generation Integrated Simulation of Living Matter" executed concurrently with the "K" computer development project, the simulation software for continuum mechanics systems (fluid dynamics, structural dynamics, etc.) and quantum systems, particle systems, and meso-level systems of computational physics and computational chemistry has been sophisticated.*

*The HPCI strategic area based mainly on the application of “K” includes 1) predicting life sciences, medicine, and chemical creation infrastructures, 2) creation of new materials/energies, 3) prediction of global climate change to prevent or alleviate disasters, 4) next-generation manufacturing, and 5) the origins and structures of matter and the universe. Of these, 2) and 4) concern the iron and steel industry. As the strategic bases in field 2), it has been decided that the Institute for Molecular Science, National Institutes of Natural Sciences and the Institute for Materials Research, Tohoku University, led by the Institute for Solid State Physics of the University of Tokyo, form centers of study for property of matter, molecules, and materials. The Institute for Materials Research, Tohoku University is the K Computational Materials Research Initiative (CMRI) for computational materials science. There, computational science regarding the development of steel materials is evolving.*

*In the “Elements Strategy” project of the Ministry of Education, Culture, Sports, Science, and Technology and JST’s industrial-academic research program “Heterogeneous Structure Control: Toward Innovative Development of Metallic Structural Materials,” there are high expectations that the mechanisms of the functional manifestation of the individual elements will be clarified by information about electronic structures in terms of space and energy obtained by first-principles calculations, that the problems of elements (resources) will be solved by the replacement of rare elements with more common substitutes, and that the processes involved in the formation of nano- and heterogeneous structures and the mechanisms manifesting their functions will be clarified by meso-level simulations using PF/MC methods, and thereby new materials having innovative functions will be developed.*

*Looking at technological developments overseas, especially the application of computational science for the development of new steel materials, not only continuum mechanics but also multiscale, multiphysics simulations at the electron-, atom-, and meso-levels are active. At present, the author has a special interest in the development of the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) at Ruhr University, Germany; the Hero-M Project (Multiscale Engineering Design) at the Swedish Royal Institute of Technology; the same kind of activities in the Max Planck Institute (Dusseldorf); the Materials Technology Lab/Steel Research Group of Northwestern University, U.S.A.; and the Center for Computational Materials Design (CCMD) at Pennsylvania State University. In the Materials Genome Initiative for Global Competitiveness of the United States, emphasis is placed on computational technology, experimental technology, and data management as the infrastructure for materials development. This program is considered to have the same concept as the “New Elements Strategy” being planned by the Japanese Ministry of Education, Culture, Sports, Science, and Technology. Also worthy of note is the program for fostering talent in the field of computational materials science of the Doctoral Training Center for Theory and Simulation of Materials (DTC-TSM) at the British Imperial College.*

*Also, in Japan’s High Performance Computation Infrastructure (HPCI) efforts are being made to create an environment allowing open access to a network of large computers at universities and businesses, including K, to expand the computational science software described above and foster personnel in the computational science field. In the iron and steel industry, we would like*

*to make great strides forward by taking this opportunity to fully utilize HPCI. Computational materials science has a multiphysics, multiscale characteristic. However, it must not necessarily allow for across-the-board simulations at all levels. What is important is to make the most effective use of the ever-expanding computer capacity to obtain the knowledge necessary to clarify the mechanisms of elementary processes of materials' behavior simply through an analysis of physics or scale of a specific hierarchy, or through, for example, data-communication-type simulations linking knowledge obtained at an atomic-level calculation to a calculation on a continuum mechanics level or a two-level hybrid simulation. With the exception of analyses based on continuum mechanics and computational thermodynamics, it cannot be denied that electronic structural analysis, molecular dynamics, and MC/PF simulations in the past were sporadic attempts to use analytical models. In the future, it is expected that these, together with particle method computing, will be applied in earnest to practical materials.*