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Utilization of Advanced Scientific Computation in Developing Materials and Processes

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Abstract:

Increasing speed, capacity, and cost performance of computers are encouraging the analysis and control of material manufacturing processes by scientific computation. The use of simulation is also expanding as a means for predicting the functions of not only conventional pure materials but also of more complex, applied materials. It is hoped that the development of computational infrastructure such as numerical computation techniques and parallel computing languages will allow utilization of advanced scientific computation to facilitate the systematic and effective use of empirical findings, enable virtual experimentation to replace actual experimentation, and to explain and predict phenomena concerned with material and process design.

1. Introduction

When the yearly performance improvement of computers is examined, it is clear that minicomputers, mainframe computers, and supercomputers have all improved in performance by one hundred fold between 1970 and the early 1990s[1]. The improvement of microprocessors since 1985 has been exceptional, with their performance increasing ten times every four years[1]. In recent years, the performance of supercomputers has improved at nearly the same rate owing to the use of multiple processors. Supercomputers operating at a few hundred MFLOPS cost several ¥ billion in 1985, whereas engineering workstations (EWS's) running at two GFLOPS cost less than ¥100 million in 1995. These figures indicate that the cost performance of computers improves tenfold every five years.

Against the background of increasing speed, capacity, and cost performance of computers as noted above, computer languages, computational techniques, and other software areas have been developed to fully use available computer capacities, and have achieved many advances. Of particular note is the fact that the ending of the Cold War has released military software for civilian use and diverted the efforts of many of the software developers engaged in military computation into general scientific computation. **Table 1** shows noteworthy topics discussed at the tutorial seminars of the 1993 Physics Computing Conference organized by the American Institute of Physics in May 1993. Many of the tutorial seminars were presented by U.S. national research laboratories that are conducting innovative numerical computation and parallel computation techniques.

Among the wide-ranging advances accomplished to date are strength design of structures and numeical wind tunnel experimentation based on continuum mechanics; macroscopic analysis of material manufacturing process behavior by the combination of continuum mechanics models with phenomenological models; microscopic analyses of mechanisms and properties where simulated are phenomena, processes and materials on the levels of atomic movement and arrangement ; and prediction of magnetic, electrical and optical properties — or, reactivity and interatomic bond strength — based on the spatial distribution and energy structure of electrons and spins. With these achievements, com-

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putation is now highlighted as the third scientific approach after theory and experimentation. This paper considers the significance, present state, and future outlook of the utilization of advanced scientific computation.

2. Significance of Scientific Computation

The significance of scientific computation in developing materials, processes, and equipment is summarized in **Fig. 1**. Firstly, in substituting for experimentation and prototype testing, computation can reduce the number of test conditions required, thereby shortening the development lead time and reducing the development cost. Next, computation can be performed under extreme environmental conditions or conditions difficult to simulate by experimentation, such as ultrahigh temperature, ultrahigh pressure, ultrastrong magnetic fields, and exposure to nuclear radiation. Computation can also be used to extensively investigate the behavior of processes, materials, and equipment under such extreme conditions, and to find optimum solutions outside the realm of conventional thinking. Furthermore, phenomena, as well as material and process behaviors and states that cannot be experimentally observed can be simulated by computation to clarify the mechanisms at work to accomplish control or optimization based on such mechanisms, and eventually to discover the seeds for developing innovative technology. For example, the spatial distribution and energy structure of electrons and their change with time, and atomic structures and their changes cannot be experimentally observed except in extremely limited portions. These phenomena, however, can be observed in detail by energy band computation according to the first-principle method, by molecular orbital computation, and by simulation with molecular dynamics and the Monte Carlo method. These computational techniques have proved effective in predicting the physical properties of materials and understanding the essence of phenomena as already described. Lastly, the computer's power is used to combine and run models for overall simulation to their end. The results of computer simulation are compared with the results of experimentation under various conditions. The models are improved until there remains no contradiction between the simulation results and the experimental results. In this way, universal models can be built and validated, and empirical findings can be utilized as technical data with high transferability, and accumulated for future use.

To put it another way, scientific computation either must allow the properties of materials and the behaviors of processes to be predicted without any empirical findings or it must provide rational methods for predicting the properties of materials and the behaviors of processes in hitherto unexperienced areas by interpolating and extrapolating empirical findings.

3. Present Utilization of Scientific Computation

Application examples of scientific computation at Nippon Steel are shown in **Fig. 2**. Continuous casting, plastic working, and plastic forming processes are the main subjects to which scientific computation is applied. Fluid dynamic analysis based on continuum mechanics and structural mechanic analysis is the predominant application technique, followed by electromagnetic field analysis, heat transfer and diffusion analysis, and thermodynamic analysis using thermodynamic models. These subjects are treated in this paper. In the materials area, attempts are being made to simulate phase diagrams, to simulate phase transformation in combination with transport phenomena, to simulate the trans-

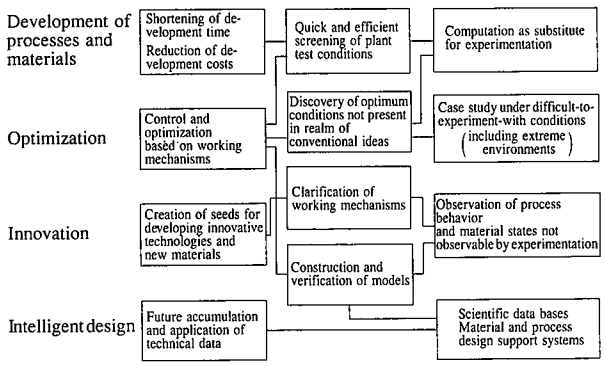

Fig. 1 Aims of scientific computation

Table 1 Tutorial seminars at 1993 Physics Computing Conference

1.Numerical computation technique		Organized by
1) Numerical fluid dynamic technique "Moving Finite Elements"	Adaptive remeshment to meet specific computational purpose.	Los Alamos Laboratory
2) Numerical fluid dynamic technique "Flux-Corrected Transport Algorithm"	Suited for parallel computation of compressible fluids, reactive fluids, multi-phase flow, turbulent-laminar flow transition, and complex-shaped flow	Naval Research Laboratory
3) Particle system simulation method	Molecular dynamic method	AEA of United Kingdom
4) Application of finite element method to quantum mechanics	Solution of wave equation by FEM	Worcester Polytechnic Institute
5) Conjugate gradient method	Solution of optimization and minimum/maximum value problems	Lawrence Livermore Laboratory
2. Parallel computation		**Organized by**
1) Parallel computer FORTRAN "High Performance FORTRAN"		Rice University
2) Massively parallel computing method "Massive Parallel"		Lawrence Livermore Laboratory
3) Parallel computer FORTRAN "Modular FORTRAN"	Provided with functions similar to those of C language and usable for data bases	Argonne National Laboratory
3. Others		**Organized by**
1) Distributed scientific computation with different makes of computers		Lawrence Livermore Laboratory
2) Programs available for use in such areas as physics, science, engineering, and mathematics		Lawrence Livermore Laboratory

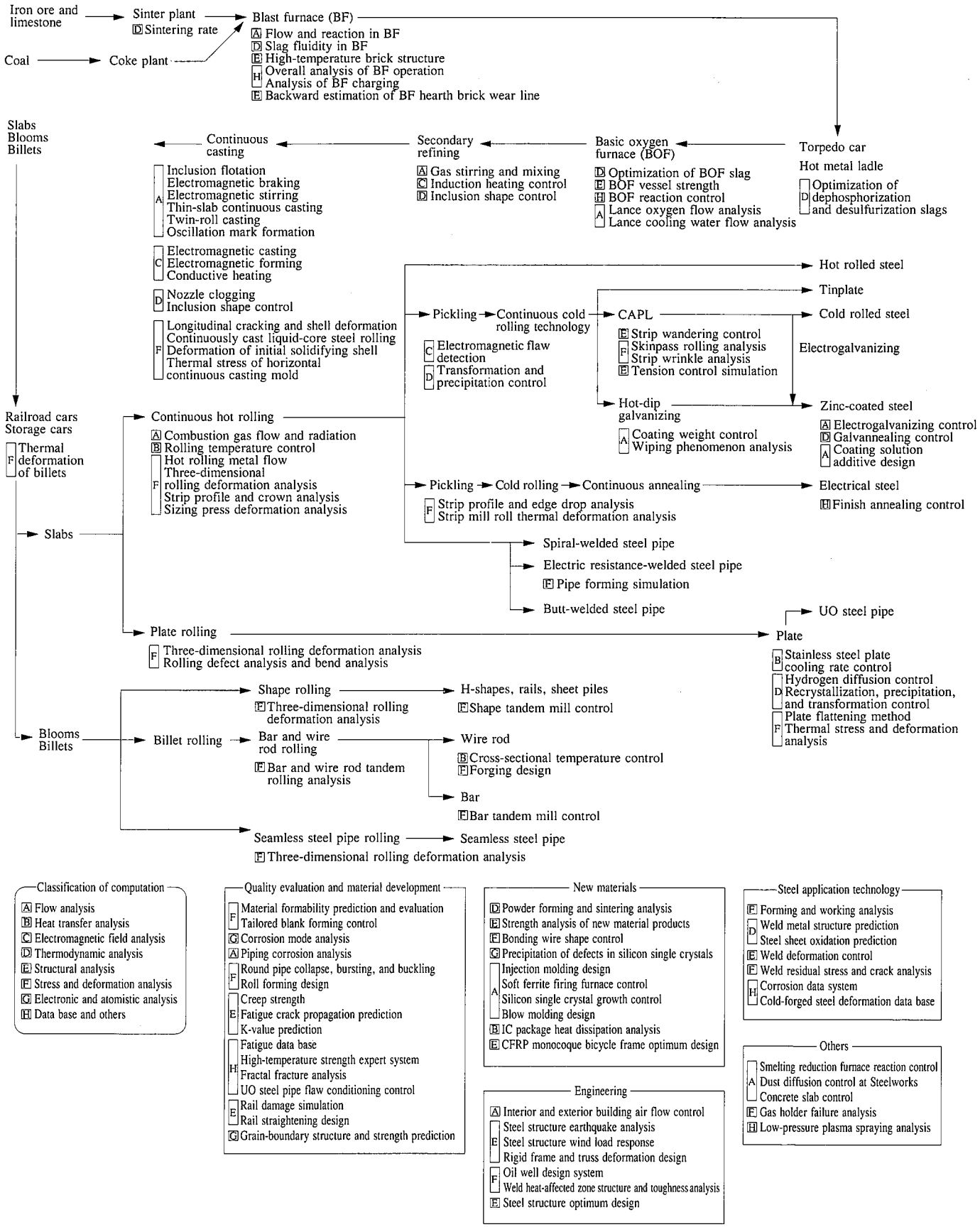

Fig. 2 Map of application examples of scientific computation

formation and recrystallization structure evolution processes by the Monte Carlo method, and to predict phase stability, grain boundaries, defects, magnetic properties, and mechanical properties in atomic and electron level analysis. These applications are still limited and are not treated here.

Problems associated with the continuous casting process include the control of nonmetallic inclusions, prevention of cracks, and suppression of center line segregation. For example, the phenomena associated with the first two problems, the elementary process models for these phenomena, and the basic equations governing these phenomena are summarized in **Fig. 3**. These phenomena are mostly divided into the elementary processes concerning the flow of molten steel, equilibrium of stresses, transport of energy and solute, electromagnetic induction, and chemical reaction. They are solved by the equation of continuity, Navier-Stokes equations, transport equations, Maxwell's equations, mechanical equilibrium equations, thermodynamic equilibrium equations, and chemical reaction rate equations. Scientific computation is applied to predict how the levels of typical cast steel defects will change with operating conditions and to study the optimum operating conditions of continuous casters. The plastic working and forming processes are simulated to investigate the assurance of dimensional accuracy and the establishment of operating conditions as required for the prevention of such defects as cracks.

4. Future Outlook of Scientific Computation

Under the present circumstances noted above, scientific computation is mainly applied to the simulation of material behavior in material manufacturing processes. These applications are often limited to the establishment of conditions for meeting qualitative, dimensional, and geometrical requirements. Future targets are virtual experimental laboratories and virtual factories for creating new materials (see **Fig. 4**). To this end, it is necessary to: 1) develop data bases containing the basic properties of materials or the scientific computing techniques for predicting the basic properties of materials; 2) develop simulation techniques — or knowledge databases — for relating basic properties, microstructures,

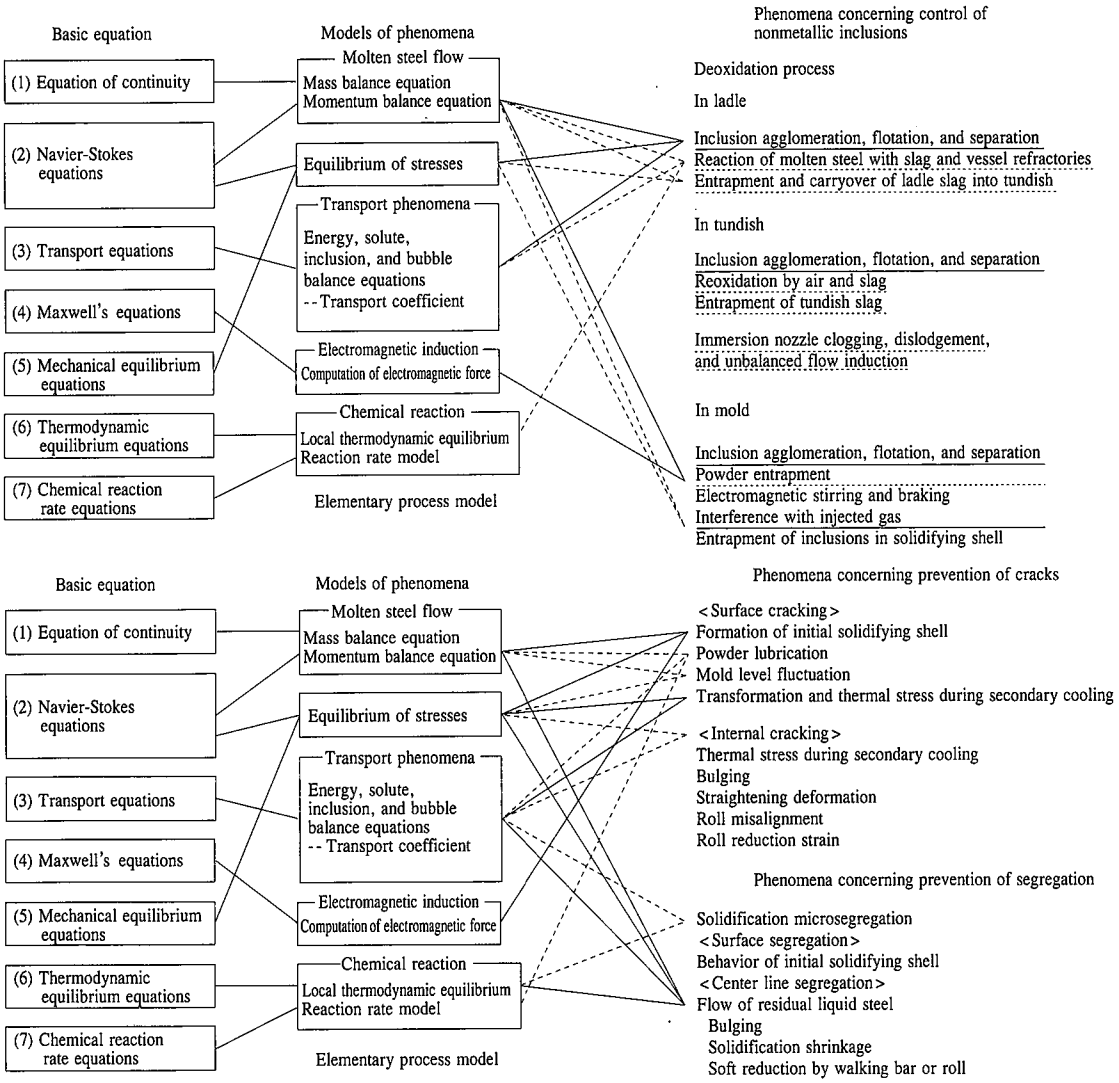

Fig. 3 Phenomena in continuous casting, and their models and basic equations

and high-order structures to performance; and 3) develop process simulation techniques for predicting the microstructure and higher-order structure of materials to be produced, or build knowledge databases for directly relating process conditions to material microstructure, higher-order structure and performance.

The scientific computing techniques in category 1) cover the analysis of electronic structures and the simulation of atomic-level material behavior by the molecular dynamics and Monte Carlo methods, and are considered not as difficult as the simulation techniques in categories 2) and 3). As far as category 2) is concerned, it will not be possible in the near future to analyze all the phenomena concerned at the electronic and atomic levels by simulation techniques, despite the marked increase in computer performance. To achieve this task, it will be necessary to apply continuum mechanics at the mesoscopic level, to develop mesoscopic-level simulation techniques through application of the

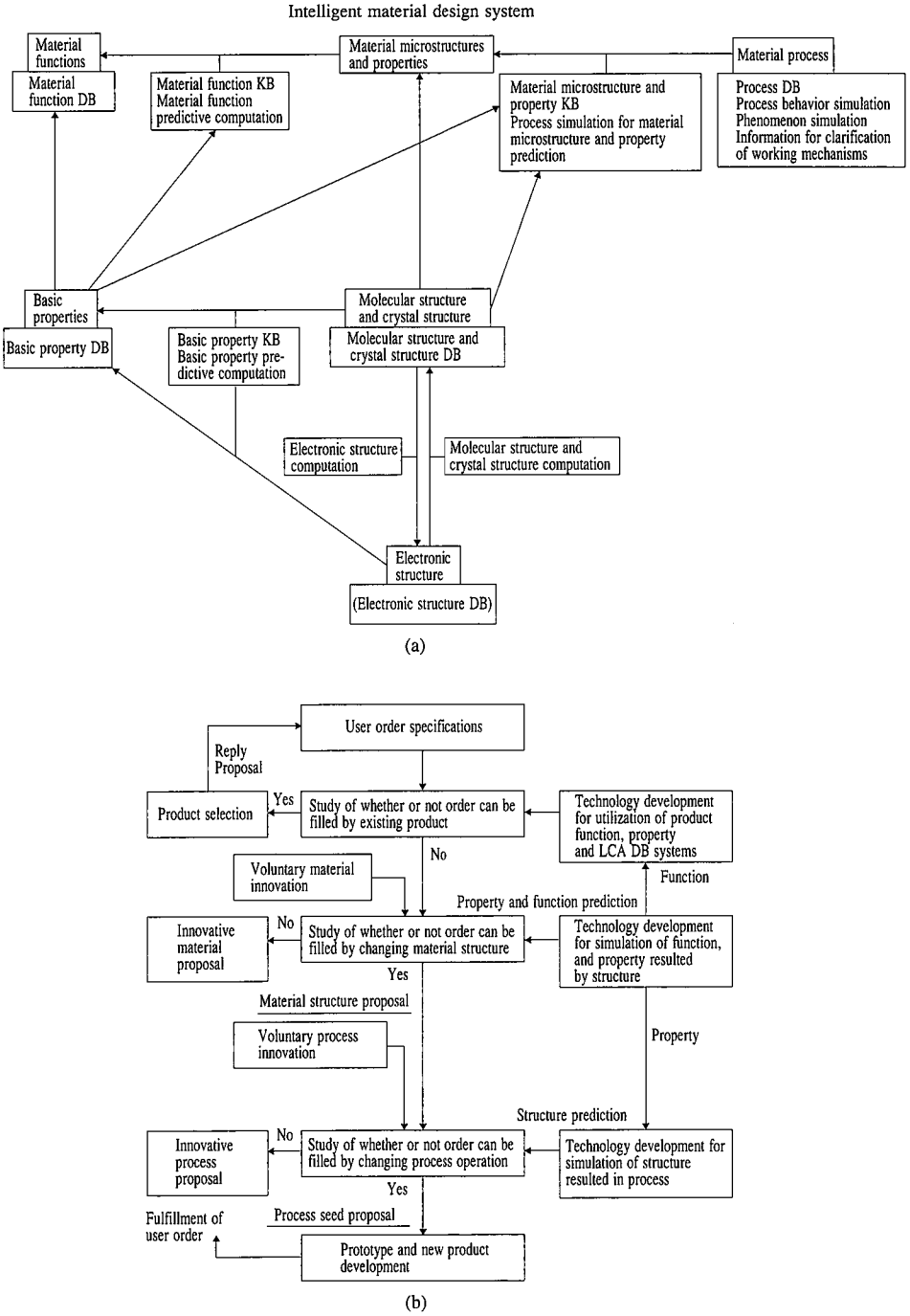

Fig. 4 Position of computational science in intelligent material design system (a) and schematic of intelligent material design system to meet social needs (b)

Monte Carlo method, and to develop hybrid simulation techniques combining continuum mechanics and atomic-level simulation. If an empirical data base of material functions is built by clarifying chemical compositions microstructures, and higher-order structures, it can be directly used as an aid in material selection and design. Among such examples are corrosion, strength, and creep data bases. As for process simulation in listed in category 3), the simulation techniques required will be able to clarify process conditions for creating material microstructures and higher-order structures similar to predicting the grain size of steel sheet to estimate its mechanical properties.

The conventional prediction of mechanical properties involves the calculation of working thermal history and the prediction of the grain size or strength of a steel of given chemical compositions from an empirical data base constructed from experimental results. The general-purpose prediction of mechanical properties without repeating such experiments for specific types of steels calls for the development of computing techniques corresponding to the simulation techniques used for computing the grain size of steels and the tensile strength of steels from their grain size. If computational science is put to effective use in making empirical data bases more augmented, generalized, and universal for predicting the physical properties of materials and predicting the functions of materials from their basic properties and conditions as described in chapter 2, new products and processes can be more rationally developed to meet social needs (see **Fig. 4**).

Lastly, it is hoped that many researchers will make direct use of computed results as shared information when they interpret the mechanisms controlling the appearance of properties and governing phenomena according to the new information obtained from scientific computation. Now that scientific papers can be contributed through computer networks, the attachment of detailed computed results as appendices is expected to allow the knowledge of many researchers to be shared and to accelerate the progress of intelligent materials design.

The map of application examples of scientific computation in **Fig. 2** has been prepared in cooperation with the members of Nippon Steel's Research Group on Advanced Utilization of Scientific Computation. The author would like to express his appreciation for that.

Reference

1) Nikkei Electronics. (546), 250 (1992)