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Structural Materials as Fundamental Technology for the Realization of Social Innovations

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Abstract

Among the consecutive arguments for the Science and Technology Innovations by the government and the agencies, the structural materials are recognized as the key factor of their promotions. It is no doubt that when the remarkably unique ideas and technologies are accepted for the actual utilizations possessing their shapes or structures, the steel products are indispensable as the typical material for the purpose. On the other hand, a lot of basic research fields are found to be remained where essential solutions are not obtained yet. It is emphasized that the appropriate research targets ought to be extracted in those field, afterwards their results can achieve the development of the most advanced steel products.

1. For the Sustainability of Social Innovations

Discussion on innovation creation in Japan, especially during the period when the Fifth Science and Technology Basic Plan was formulated, has been extensively undertaken among the Government and Agencies, together with private organizations such as the Federation of Economic Organizations ^{1,2}. Needless to say, we have experienced a multitude of innovations generated through economic development in the past several decades including the early post-war days, and expect innovation to continue in future as well.

Whenever societies advance driven by innovative science and technologies, or by novel ideas, appropriate structural materials are sought at the final stage of the realization of their characteristics and structures. Steel products, as a representative material, have always satisfied the needs of society, and efforts have been made to enhance their performance through either cooperation or occasionally with other competing materials. Such steel products embody unexpectedly developed "objects" and provide them with form; therefore, the performance required of them cannot be realized with conventional technology. In most cases, fulfillment toward satisfying such needs is only finally achieved narrowly as a result of strenuous efforts to determine unprecedented performance.

By studying the history of the models described above, one may find the characteristics of the steel products that become hardened after a forming process³⁾ while remaining soft in the manufacturing process and or, the realization of deep-drawing of a blank flat sheet to form a long and narrow can⁴⁾. Cases are varied. There may be a case in which the performance of another raw material is realized by steel and or, a case in which the performance, specific to steel only and made feasible only by steel, was thoroughly explored to its ultimacy upon the requirements of users.

Steels possess unique characteristics and even now, by combining such characteristics in various manners, new characteristics are continuously being developed and realized to satisfy new requirements, such as corrosion-free steel for marine constructions⁵⁾ and steel that changes its crystalline structure at the stage where its users use the steel³⁾. How were such new characteristics realized? Some may have been achieved afresh by probing deep into and clarifying the characteristics that had been disregarded or ignored or, there may have been a case in which a performance, overlooked by someone previously, has been constructed uniquely as suggested by a physical property table.

In short, steel has many unclarified fundamental properties including physical properties. Even the physical mechanism of the utmost fundamental transformation of the α phase to γ phase has not been sufficiently clarified, and the behavior of the yielding point in a tensile strength test has still not been established among various theories. Furthermore, the dynamic behaviors and the atomic structures at grain boundaries of lattice defects such as dislocation during plastic deformation still linger in the model-concept area. Complete clarification of such phenomena is not necessarily required; however, to develop steels with new performances, it is essential to add even the slightest piece of new knowledge to the conventional tech-

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nologies that have long been accumulated to date.

The production amount of iron and steel in Japan has remained stagnant at its apex for the past forty years. On the other hand, from the global viewpoint, it is still a market field where future growth on a long-time span is expected. In reality, most steel products of commercial quality that were previously produced in Japan are now produced by developing countries, which are contributing to extending the boundaries of the steel market. In such a market, the Japanese steel industry continues to produce one hundred million tons of steel in the summit area of the quality hierarchy where steel performance is incessantly upgraded. In the schematic structure, to comply with the social needs that are considered to increase in future as stated at the beginning, and to realize the enhancement of the performance of steel products, it is absolutely essential for the iron and steel industry in Japan to clarify the fundamental base metallurgy that has not yet been elucidated, and utilize the results obtained.

2. Structural Materials for Forming Strong Steel Products

The function of structural material is to generate and to maintain the form. Its critical function is simply represented by strength that is the resistance ability against deformation and toughness to prevent fracture. The actual phenomena, to which structural materials are exposed, are exceedingly varied.

Deformation is categorized by mode, namely reversible elastic deformation and irreversible plastic deformation. Although they differ according to their physical properties, they are often discussed as a single consistent serial phenomenon in the development of materials. Development of the most advanced materials requires accuracy in the forming of high tensile strength materials, deformation resistance and temperature resistance for impact deformation in cars, ships, architectural structures, etc. (**Fig. 1**⁶).

Although various macroscopic behaviors of fracture are well arranged and classified and the comprehension of the phenomena is widely prevalent, clarification of the mechanism based on the true nature of material remains insufficient. Propagation of a crack, for instance, may primarily be the continuation of fracture of atomic binding. However, atom level fracture has never been observed on a cleavage fracture surface. Crack propagation is always accompanied by a very minute plastic deformation region formed at the crack end and signs of some mitigating phenomenon on the newly emerging surface are also found. More macroscopically, a certain degree of dissociation exists between the direction of fracture stress and the direction of cleavage. Occasionally, a ductile fracture region linking across both cleavage planes exists that seems to act by mitigating the dissociation. Even when a fracture shows brittle fracture mode macroscopically, microscopically, fracture is developed by a combined process of brittle fracturing and ductile fracturing (Fig. 2⁷).

In the actual usage in society, in order for structural materials to be furnished with functionalities, characteristics to secure reliability in fatigue-fracture resistance, wear resistance, etc. are also important. Most probably, if the phenomenon is analyzed and reviewed on a fundamental basis, these modes of fracture are the combined phenomenon of the abovementioned elasto-plasticity deformation and the ductile brittle fracture. Furthermore, another subject is how to describe precisely the characteristics as the result of overall analysis, taking into consideration the elapse of time and the thermal hysteresis. Furthermore, by taking into consideration the chemical reaction between a material and its environment, other characteristics such as corrosion resistance can also be described.



Fig. 1 Strain stress curves of polycrystalline steels at -18°C⁶



Fig. 2 River patterns observed on the brittle ruptured surface 7)

The characteristics of steel products allow the existence of not only the basic phase of BCC: ferrite alone, but also a mixture of various phase microstructures developed by the addition of a very small quantity of elements and or by heat treatment such as FCC: austenite, carbide: cementite, semi-stabilized BCT: martensite, etc. Many of the characteristics are not simply the sum of the characteristics of the respective phase, but in many cases, are determined by the effect of the distribution state of the respective phase. Most of the efforts in the conventional research and development have been dedicated to the control of microstructures.

Nowadays, the steel products market has been hit by rapid globalization within a very short period of time and therefore, a direct link between the development of commercial products and material research is being sought more strongly than ever before. Therefore, it has become more important than ever to return to the fundamental base of research and deepen our basic knowledge and execute immediate feedforward to material designing.

3. Fundamental Approach of Basic Study on Polycrystalline Material Conducted from Elasto-plasticity Viewpoint, as an Example

Amongst the various uses of steel products that range from several millimeters to several kilometers in terms of length alone for instance, metallic microstructures are always microscopically constructed of uniform crystalline grain microstructures of several micron meters to several tens of micron meters. Functions such as strength, toughness and formability are provided by polycrystalline grain microstructures persistently and the roles of elastic deformation and plastic deformation developed in a polycrystalline microstructure are studied once again.

The dynamic behavior of lattice defects represented by dislocation is considered to appear within a crystal grain as if the grain is a monocrystal grain. However, sometimes it happens that the adjacent crystal grain has a different crystalline orientation or, has a different crystalline system depending on the individual case. Physical properties are discontinued there and the crystalline grain boundaries bear the stress caused by the dissociation. The local strain thus accumulated at the grain boundaries is expected to enhance strength and toughness, etc. as a result thereof. However, not many studies have been conducted that explain the mechanism of strain by separating elasticity from plasticity or vice versa.

Strain accumulated at grain boundaries is not uniform (**Fig. 3**); however, it is not always disorderly either. When the deformed microstructure in the neighborhood of a grain boundary is observed, several characteristic forms are observed. The periodically distributed band structure creates the repeating orientation fluctuation possessing some orientation relationship, suggesting the apparent activities of specific slip systems. Sometimes the "penetration" of similar deformation microstructures to adjacent crystalline grains is observed, however, not frequently. Ultimately, as the continuity in plastic strain such as this form is maintained only when the geometrically consistent orientation relation is maintained, it is common that the continuity is generally disrupted at grain boundaries. Then, it is considered that, in the adjacent grain where plastic deformation has not been realized, elastic strain is developed and the stress so produced acts as an external force to the grain.

Now plastic strain is reviewed from the textbook viewpoint^{8,9)}. The fundamental unit of lattice defect and or dislocation forms a heterogeneous elasticity field according to the formed lattice strain, the field of which accumulates energy and develops interactions among lattice defects. This means that what forms a field of strain is

a field of elasticity and not plasticity itself. ("Field of elasticity" exists but "Field of plasticity" does not exist.) Accordingly, the strain accumulated at grain boundaries is primarily of elastic strain. Plastic strain is considered to be either what appears as a result of mitigation when geometrical conditions are orderly consistent, or a group of dislocations that has remained in the neighborhood of grain boundaries as the residue of plastic deformation. No matter what the case, the strain energy that appears there is "elastic".

Another example of elastic strain accumulated at grain boundaries is introduced. **Figure 4**¹⁰ shows the structure obtained when bicrystal consisting of $\{100\} < 011$ oriented grains that are most susceptible to the rolling deformation in BCC steel and the grains with the same orientation are tilted by several degrees as to the rollingdirection (RD), wherein the crystalline grain boundaries are oriented in the rollingdirection. Despite plain strain considered to be devel-



Fig. 3 Microscale strains accumulated at the grain boundary



Fig. 4 Observed elastic strain besides the grain boundary¹⁰

oped herein, moderate strain in the transverse direction as to the direction of rolling (TD) is observed near grain boundaries. This is an example whereby slips within grains of both are discontinued at grain boundaries and the extent of discontinuity is mitigated mainly by elastic strain.

More precisely, both $(110)[\bar{1}11]$ and $(1\bar{1}0)[111]$ slips are required to be activated simultaneously to realize the steady orientation of (100)[011] grain under the plain strain condition during cold rolling. Assuming these slips are employed with the screw dislocations, they can move across each other. However, when the actual crystalline orientation deviated slightly from (100)[011], orientation of elongation of the sheet deviates from the direction of rolling and, another strain introduced so as to alleviate the deviation is accumulated at the grain boundaries. To realize the mitigation of the strain with slip, in the case of Fig. 4, $(101)[\bar{1}11]$ slip has to be activated. However, the screw dislocations that glide over the slip plane described above cannot cross both dislocations. Consequently, the elastic strain ought to be mainly contained instead of plastic strain to maintain the volume continuity. Therefore, in the strain where elasticity is the major component, continuity in volume has to be secured.

When heat treatment is applied to the strain microstructure, crystalline orientations unpredictable from the slip system are developed in recrystallization (Fig. 5¹⁰). In the case that the accumulated strain is assumed to be elastic in nature, what sort of thermal release process is considered? Elastic strain caused by the restraining of the adjacent grain is maintained because the restraining force is below yielding strength. Accordingly, in the case that the yielding strength is lowered by heating, the restraining force or stress can exceed the yielding strength, and "buckling" takes place consequently. The transformation of the elasticity strain to plasticity strain mode is considered to take place. If the new orientation developed by the buckling is of low strain microstructure, it may achieve entire recrystallization, encroaching on the surrounding deformation microstructures. Although the abovementioned mechanism has been rarely discussed in the research on recrystallization, it may not necessarily be an illogical concept when discussed from the viewpoint of the fundamental basis of material deformation. As a matter of course,



Fig. 5 Recrystallization at the grain boundary where elastic strain was piled up ¹⁰

sufficient verification as to what type of orientations can exist after buckling is required. However, due to space limitations, this subject remains a topic for future discussion.

4. Steel Technology, a Treasure House Richly Filled with Subjects of Fundamental Basic Research

To date, for the understanding of strength and toughness of steel products for use as structural materials, discussions have been mainly based on elasto-plasticity theories. However, even though elastoplasticity theories are acknowledged as the foundation of the study, in reality, material science and technology consist of various physical properties' theories and kinetics, overlapping each other. Among the discussions, some seem to refer to material properties (= performance), some to the production process (= process) and some to fundamental basic analysis (= principle) with the intention of applying them, and contributing to material design. Figure 6 shows the mapping of the subjects considered to be tackled by the iron and steel industry. This was realized as a result of the discussion in the iron and steel subcommittee of the Innovative Structural Materials Project (ISMA) promoted by the Ministry of Economy, Trade and Industry and the New Energy and Industrial Technology Development Organization (NEDO). Without solving all the several tens of subjects listed therein, not even a single piece of steel sheet can be produced. Furthermore, each subject interacts closely with the other, and for the creation of new material properties, clarification of the principle by means of fundamental basic analysis is indispensable. This means that the incessant back and forth flows of the outcome of research and development between the fundamental basic research and the application fields is essentially required for the enhancement of the quality and the speed of the developing process of new products.

On the other hand, as described so far, in steel products, even today, there are still several subjects that have to be pursued from the viewpoint of a fundamental research base. This aspect is discussed, quoting the discussion result in the "Elements Strategy Initiative <Core Research Centers>"11) administered by the Ministry of Education, Culture, Sports, Science and Technology. Japan has high potentiality in the material industry, and even though a new product market is created in a foreign country in line with the emergence of a new state of living in the country, parts and or the materials are supplied by Japan in many cases. Figure 7 shows the results of arrangement of the following items: development of new products therefore, linkage thereof to fundamental basic theories that bear the new product, systemization of the flow from the stage of developing parts and or primary materials to the steps of arrival at end users in the form of finished goods and building-in in construction. Electronics or the like, which once drove the industry and the economy in Japan, is the field where the creation of new substances based on fundamental physiques is directly linked to the development of new electronic devices. However, in the field of structural materials, the tie between the structural materials and the construction of structural members is relatively strong and, in order for the outcome of the research based on fundamental basic theories to be linked to structural materials, several obstacles have to be cleared. Furthermore, the separation distance reaching an end user is unexpectedly far when compared with the case of other primary materials and there still exist many users' needs that can be considered in fundamental basic research.

The same applies to steel products. The actual outcome of various product developments that have been realized through deepened

Characterization	Properties	Performances
Crystal structure	Chemical contents	Toughness
Crystal system / Crystal anisotropy	Solution	Low temperature toughness
Atomic bonding / State of electron	Segregation	Impact toughness
Grain boundary / Twin boundary	Phase separation	Joining toughness
Vacancy / Dislocation	Metastable phase	Notch toughness
Slip system	Interstitial / Substitutional	
Coherent strain	Inclusion	Strength
Lattice strain	Microstructure	High temperature strength
Thermodynamics / Free energy	Grain size	Yield strength
Precipitation	Phase equilibrium /	Work hardening
Interface energy / Interface reaction /	Phase partitioning	Rupture strength
Phase transformation	Recovery / Recrystallization /	High elasticity
Metastable phase /	Grain growth	Joining strength
Strain induced phase transformation	Residual stress /	T 1 114
Suam mudeed phase transformation	Stress distribution	Formability
Kinetics	Texture	Rupture strain
Diffusion	Interface	Press formability
Phase transformation rate	Ovidation / Nitriding /	Joining property
Precipitation rate	Sulfidation / Decarbulization	Machinability
Casting / Grain boundary migration	Tribology / Friction	Forging
Stress response	Joining interface	Reliability
Elastic field	Heterogenouse interface	Fatigue
Elastic compliance	Interface shape / Roughness	Corrosion resistibility
Yield / Critical share stress	Puntured surface / Creak	Heat resistibility /
Metal flow	Ruptured surface / Crack	Creep property
Flomonts function	Crack propagation	Time deterioration
Light elements / Hydrogen	Stress distribution /	Stress corrosion cracking
Lattice vibration / Phonon	Stress concentration	
Magnetism	Elasticity /	
Pare elements substitution	Plastically deformed distribution	
Kare ciements substitution	i modeliny deformed distribution	

Fig. 6 Subjects in the basic metallurgy for the development of the steels



Fig. 7 Both directions towards the basic filed and the application field from the materials viewpoint¹¹

exploration into fundamental basic theories as a trend and tight dialogue with users is owing to the large gaps remaining in the fundamental basic theory field and the actual application field that allow and accept further extensions of the product development in either direction into the fundamental basic field or into the application field. Actually, in the direction of the fundamental basic field for instance, remarkably increasing is the share of utilization by the industry of large-scale research facilities constructed by the government such as J-PARC with a powerful quantum beam emitter and Spring-8, an analysis facility using synchrotron radiation¹²⁾. Unquestionably, in structural material research, bulk analysis and insitu observation have been insufficiently conducted, and such research is considered to be very effective in future. A research method exceedingly more efficient than the conventional research methods is expected for shape-forming analysis and or the evaluation of reliability in actual application fields.

5. Conclusion

The mission of the Fundamental Metallurgy Research Laboratory in Nippon Steel & Sumitomo Metal Corporation is not simply to conduct deeper basic research. To clarify and to show how a research can be linked to social needs of materials, to identify the subject that needs to be extensively researched amongst a series of development stages integrated like a supply chain, and to dash forward to the solution of the research subject so extracted ought to be its essential role in R & D Laboratories. The outcome of the research should be definitely transferred to the development of new products; consequently, it must be provided to survive and conquer the competition in the market of most advanced steels that is growing increasingly harsh.

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