Giant Straining Process for Advanced Materials Containing Ultra-High Density Lattice Defects

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We have started a new research program supported by a Grant in Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology (so called Monbusho Grant). The category of the program is in the Priority Area with the program title "Giant Straining Process for Advanced Materials Containing Ultra-High Density Lattice Defects", beginning in September 2006 and ending in March 2009. We periodically issue News Letters as a part of activity of this program.

It is well known that severe plastic deformation (SPD) is an important process for microstructure refinement. ECAP (Equal-Channel Angular Pressing), HPT (High Pressure Torsion) and ARB (Accumulative Roll Bonding) are typical processes for SPD. These SPD processes are capable of reducing the grain size to the submicrometer or nanometer range. Dispersion of second phases to the nano or atomic scale is also feasible with the SPD processes. An attractive feature of the SPD processes is that the dimensions of the cross section never changes through deformation and this is very unique as other conventional processes like rolling, extrusion, drawing etc. do change the dimensions. Because of this unique feature, intense strain is introduced in the sample. Since the strain is enormous, unusual properties often appear to result in simultaneous enhancement of the strength and ductility.

Intense strain is also created on the sample surfaces using the processes of shot peening, drilling and sliding wear and in powders through ball milling especially at cryogenic temperatures. This research program includes studies not only for straining of bulk materials but also for straining of surfaces and powders. Because the SPD is a terminology used for large straining of bulk materials [1], we use instead “Giant Straining Processes (GSP)” in the title so that this program can accommodate intense straining of surfaces and powders.

Now, generally what happens to the materials if strain is imparted? The answer is very obvious. Many lattice defects are generated in the sample. Here, the lattice defects include vacancies, dislocations, stacking faults, twins, grain boundaries, etc. and it is these lattice defects that determine the properties of the materials. A question is what happens if the strain is too much? We know that grain size is significantly reduced. However, we don’t know why it is reduced. Although the GPS provides unique properties, information is very limited why mechanical properties are enhanced in terms of both strength and ductility. This is a main motivation that this research program has been initiated.

It is reasonable to consider that lattice defects created by GPS have a close relation to the grain refinement and subsequent improvement of mechanical properties. Objectives of this research program are two folds. First, we examine mechanisms of grain refinement when large strain is imposed on the samples through GPS. Second, we investigate mechanisms for the unusual and unique mechanical properties that result in simultaneous enhancement of the strength and ductility.

In order to achieve the goal, this research program will be implemented with 3 teams. Each team consists of 2 groups: one is based on experimental measurements and structure observations and the other is theoretical calculation and computer simulation (see illustration). Under this scheme, the first team (A01) produces ultrafine-grained materials in well controlled conditions and simulates grain refinement behavior. The second team (A02) measures mechanical properties and investigates mechanisms for the advent of unique mechanical properties as simultaneous achievement of strength and ductility. The third team (A03) investigate roles of lattice defects on the production of fine grain structures and the unique mechanical properties. Each objective and role of the six groups is further described in the following pages.

Intense strain is produced in metallic materials using the process of severe plastic deformation (SPD) such as equal-channel angular pressing (ECAP), accumulative roll bonding (ARB) and high pressure torsion (HPT). Enormous strain is also created on metallic surfaces after shot peening and drilling and stored in metallic powders by cryogenic ball milling. This research group operates these giant straining processes (GSP) and provides the GSP samples to other research groups to investigate roles of high-density lattice defects in microstructure refinement including grain refinement and fine dispersion of second phases. GSP is operated with controlled manners so that reproducibility is maintained for the GSP samples.

Objectives of this study group are to clarify underlying mechanisms for the development of fine-grained microstructures and to understand the mechanical response of metal polycrystals with high-density lattice defects by using numerical techniques of macro- and meso-mechanics. In the macroscopic analyses, strain histories in materials processed by ARB or ECAP are quantitatively evaluated. The crystal plasticity analyses are performed to understand the characteristics and particularities of dislocation accumulations under different deformation modes. Macroscopic mechanical responses of nano-structured metals are also predicted by crystal plasticity analyses. Thermodynamic stability of ultrafine grained structures is discussed with phase field simulations.

The purpose is to reveal the mechanisms of peculiar mechanics and phenomena involved in high-density lattice defect (HDLD) materials such as yield-drop phenomena, high strength and ductility, abnormal rate-dependent deformation, fracture and toughness, etc. As experimental studies, systematic testing of mechanical properties, microstructure observation, dynamic in-situ analysis by neutron diffraction will be conducted.

Theoretical studies such as those based on dislocation theories, fracture mechanics and micromechanics will also be performed to establish science of high-density lattice defect materials.

These studies are expected to give insights into designing new types of high-strength and high-ductility materials.
The purpose of this group is to clarify the emergent mechanism of unique mechanical properties of giant-strained materials. The key concept of the methodology is on the time evolution of those internal structures consisting of ultra-high density lattice defects. We adopt simulations based on discrete models in various space and time scales, e.g., molecular dynamics, discrete dislocation dynamics, distinct element method and quasicontinuum method. New multiscale meso-plasticity models we develop here can seamlessly bridge between large-scale molecular dynamics and coarse-grained models and also can express the representative volume element and the elementary process for plastic deformation of giant-strained materials. Using the multiscale models, we determine the better internal structure of the materials, e.g., grain arrangements in a bimodal structure and the distribution of grain boundary characteristics, and propose design principles in collaboration with experimental groups.

Our purpose is to clarify the mechanism for the formation and stabilization of high-density lattice defects in severely deformed materials and also for the emergence of unique properties in them. To this end, statistically averaged information is evaluated on the strain distributions and on the high-density mobile and immobile dislocations by using diffraction technique of high-energy synchrotron radiation, and the acoustic method as well. Local information is obtained focusing mainly on the grain boundary and interface structures in them by using the high resolution TEM and the 3D atom probe. In addition, local strain is first examined from the morphological change of precipitates with severe deformation. The combined use of the information obtained from these analyses with the first-principles calculations will lead to the fundamental understanding of a whole feature of the severely deformed materials.

First-principles calculations based on density functional theory are applied to high density lattice defects (HDLD) materials such as Al or Cu alloys formed by severe plastic deformation process, and the mechanisms of novel mechanical properties and the formation process of nanostructures are investigated. Basic interactions among various defects in the HDLD materials, such as those between point defects (including solute atoms), between point defects and dislocations, between dislocations, and between defects and grain boundaries, are examined, and basic mechanical behavior of HDLD systems is simulated through the behavior of atoms and electrons, by large-scale supercell calculations. Results are closely compared with experimental studies and atomistic or meso-scopic simulations of other research groups to elucidate the mechanisms.
Hardening by Annealing, and Softening by Deformation ??

It is a common sense for material scientists that metallic materials are hardened by plastic deformation (so-called strain-hardening) and softened by subsequent annealing heat-treatment. It was, however, found that completely opposite behaviors happen in the nanostructured metals fabricated by giant straining process. The surprising results that were obtained through a collaboration between one of the members of the “Giant Straining” project (N.Tsuji, Osaka Univ.) and Risø National Laboratory, Denmark, were published in Science journal (Science, Vol.312, No.5771 (2006), pp.249-251). Pure aluminum sheets were highly strained by the ARB process, resulting in an ultrafine grained structure. When the ARB processed material is annealed at relatively low temperature, like 150°C, the yield strength obviously increased and the ductility greatly decreased, which was called “hardening by annealing”. When the hardened nano-metal is cold-rolled by 15% at RT, the flow stress significantly decreased and the ductility greatly recovered. This was “softening by deformation”. The phenomena, surprisingly, repeatedly occurred after subsequent annealing and deformation. It was clarified that the abnormal behaviors are attributed to the deficiency of free mobile dislocations in the nanostructured metals. On the other hand, it is still unclear why the dislocation sources are so impotent in the ultrafine grained microstructures, which will be a future subject to be clarified in the project. Anyhow, the present finding throws light on a new possibility to manage both strength and ductility in the nanostructured metallic materials.

Latest information

Equivalent strain for ECAP and HPT

There is much confusion concerning the equations for calculating equivalent strain in ECAP and HPT. We confirmed at a group meeting in Chiba on March 5, 2007 that the following equations are correct forms.

**ECAP**

\[ \varepsilon_N = \frac{N}{\sqrt{3}} \left( 2 \cot \left( \frac{\phi}{2} + \frac{\psi}{2} \right) + \psi \ \text{cosec} \left( \frac{\phi}{2} + \frac{\psi}{2} \right) \right) \]

\( \varepsilon_N \): equivalent strain after \( N \) passes, \( \phi \): channel inner angle, \( \psi \): channel outer angle.


**HPT**

\[ \varepsilon_N = \frac{2\pi N}{\sqrt{3t}} \]

\( \varepsilon_N \): equivalent strain after \( N \) turns, \( \rho \): distance from disk center, \( t \): thickness.


Call for papers

Special Issue of Materials Transaction (International Journal of Japan Institute of Metals)

**Title**: Severe Plastic Deformation for Production of Ultrafine Structures and Unusual Mechanical Properties : Investigating Role of High-Density Lattice Defects

**Scope**: This special issue is edited to summarize recent research activity associated with severe plastic deformation (SPD). It is well known that significant refinement of microstructure is achieved in metallic materials using the SPD processes such as equal-channel angular pressing, accumulative roll bonding and high-pressure torsion. High-strength and high ductility are also achieved simultaneously through SPD. This issue focuses specially on the role of high-density lattice defects (vacancy, dislocation, grain boundary, twin) introduced by the SPD processes for the microstructure refinement and simultaneous achievement of high strength and high ductility. Articles are included not only from experimental studies but also theoretical simulation and modeling.

**Topics**: equal-channel angular pressing (ECAP), accumulative roll bonding (ARB), high-pressure torsion (HPT), severe plastic deformation (SPD), lattice defect, vacancy, dislocation grain boundary, twin, ultrafine grained structure, high strength, high ductility

**Publication Schedule**:

Dead line for manuscript submission, July 2, 2007

Completion for paper review, November 2, 2007

Publication, January, 2008

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