Giant Straining Process for Advanced Materials Containing Ultra-High Density Lattice Defects
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http://zaiko6.zaiko.kyushu-u.ac.jp/spd/index_e.html

**Numerical insight into microstructure evolution under severe plastic deformation** (presented by A01(b) group)

Members in the research group A01(b) are performing numerical simulations for the development of ultrafine grained microstructures by severe plastic deformation, one from mesoscopic and the other from macroscopic view points. An approach by crystal plasticity analysis is going to reveal the process from dislocation accumulation to the formation of high angle grain boundaries in crystal grains. Analysis from macroscopic view point is focusing on more realistic deformation process to compare with experimental data. Comparison suggests that not only the quantity of strain but also deformation mode play important roles in SPD processes.

**[Crystal plasticity analysis]:**

A multiscale crystal plasticity model considering the evolution of dislocation structures expressed both by dislocation patterning and accumulation of geometrically necessary (GN) dislocations can computationally reproduce a production process of ultrafine-grains under the giant strain. Figure 1 shows the obtained numerical results, i.e., dislocation cell and subgrain patterns (Fig.1a,b), evolution of dense dislocation walls (Fig.1c), its transition to micro-bands and lamellar dislocation structure (Fig.1d) and formation of subdivision surrounded by high angle boundaries (Fig.1e,f). It is clarified that activation of three or more slip systems facilitates the fine-graining.

![Fig.1 Numerical results of severe plastic deformation for Cu polycrystal. (a)-(d) Dislocation density, (e) Crystal orientation and high angle boundary, (f) Dense GN dislocations.](image-url)
Distributions of strain, microstructure and hardness in caliber rolled low carbon steel bars were examined and numerically analyzed in detail*. The steel bars were fabricated by multi-pass warm caliber rolling (Fig.2(a)). Three-dimensional finite element analyses were also carried out to evaluate the distributions of the strain accumulated and the strain components introduced by each rolling pass. Numerically obtained strain distribution was in excellent agreement with experimental results of hardness distribution (Fig.2(b,c)). The area around the center consisted of a strong $\alpha$-fiber (RD//<110>) texture, while such texture was not produced in the areas around corners (Fig.2(d)). Ultrafine ferrite grains with the size smaller than 680 nm were observed in the areas around the corners. FEM results showed that equivalent strain up to 5.9 was introduced in the areas around the corners and the deformation mode was a bidirectional simple compressive one.


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**Fig.2** Quantitative correlation between equivalent strain and hardness in 7.9mm square bar after 13-pass warm caliber rolling, and EBSD maps at center and corners. (a) Schematic illustration of caliber rolling, (b) Equivalent strain distribution, (c) Hardness distribution and (d) Orientation maps along RD.
Macro- to Meso-scopic mechanical response and microstructure evolution

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Grain boundary-dislocation interaction;
Theoretical and phenomenological models for dislocation-grain boundary interactions were being developed for the prediction of macroscopic mechanical response. A higher-order strain-gradient crystal plasticity model that incorporated an influence of geometrically necessary dislocation-induced internal stresses was generalized to a finite strain theory. Effect of grain boundaries to the mean free path of moving dislocations was also studied. A basic deformation behavior in the vicinity of a single grain boundary was investigated through nanoindentation. It was clarified that a grain boundary acts as a dislocation source for the plasticity initiation and a barrier to the dislocation motion at the subsequent stage of deformation. Figure represents a TEM micrograph showing pile-up dislocations during indentation-induced deformation of a Fe-C alloy.

Development of microstructure;
Computation on ultrafine-graining was performed on the bases of evolution of dislocation structure. Using numerical and experimental analyses, quantitative correlation between equivalent strain, hardness and microstructures were made clear in low carbon steel bars fabricated by caliber rolling. [See the article on the pages 1-2.] Phase stability of metals was investigated by using a non-linear diffusion equation. Results indicated that spinodal decomposition expected to be retarded under severe plastic deformation.

HPT-processed pure Cu softened at room temperature

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Pure Cu softened when it was kept at room temperature (RT) after processing with high pressure torsion (HPT). Such softening does not usually happen in pure Cu deformed by cold rolling. As shown in the figure, the microhardness of 99.99% Cu (OFHC), which is one of the common materials in this “Giant Straining” project, exhibited Hv ~1.52 GPa after HPT with conditions of one turn at 0.2 rpm under 5 GPa. However, after keeping for 110 days at RT, the hardness decreased to Hv ~1.40 GPa at the outer regions 4 mm from the center (equivalent strain of $\text{\varepsilon}_{\text{eq}} \geq 24$). The hardness decrease was minor at the distance ~2 mm from the center ($\text{\varepsilon}_{\text{eq}} \sim 12$). This suggests that the large strain has a significant effect on the softening behavior even at low temperature. Hence, careful attention is required for the handling and the keeping if metallic materials are subjected to severe plastic deformation such as HPT, ECAP (equal-channel angular pressing) and ARB (accumulative roll bonding).
Brittle-to-ductile transition enhanced by an accumulative roll bonding process.

Masaharu Kato, Susumu Onaka (Tokyo Institute of Technology), Kenji Higashida (Kyushu University), Yo Tomota (Ibaraki University), Nobuhiro Tsuji (Osaka University), Mayumi Suzuki (Tohoku University), Yoshimi Watanabe (Nagoya Institute of Technology), Hiromoto Kitahara (Kumamoto University), Takumi Haruna (Kansai University)

In order to unveil such a mechanism that giant-strained metals exhibit high toughness at low temperatures without losing their strength, four-point bending tests are being carried out at a series of temperatures from 77K to 300K. The fracture toughness of low carbon steel at 77K is remarkably enhanced by an accumulative roll bonding process. Figure shows an outlook of the bending equipment which is set up for the project. The bending jig is surrounded by PTFE blocks and the temperature is controlled by the flow rate of cold nitrogen gas. By using this equipment, the fracture toughness of giant-strained materials is being measured over a wide range of temperatures and strain rates. The activation energy for the brittle-to-ductile transition will be obtained, which gives an insight of dislocation activity during the transition.


Microdynamics Analysis on Advanced Materials Containing Ultra-High Density Lattice Defects

Akihiro Nakatani (Osaka University), Tomotsugu Shimokawa (Kanazawa University), Takashi Matsushima (Tsukuba University), Toshihiro Kameda (Tsukuba University), and Ryosuke Matsumoto (Kyoto University)

In the group A02(d) the mechanism of mechanical properties observed in macroscopic point of view are studied through understanding the microstructure and corrective behavior of lattice defects. The members conduct not only analysing the time evolution of geometrical structures in a framework of boundary value problem in various scale levels, but linking the methodologies each other towards multiscale analyses.

The figure shows a stress distribution in the vicinity of a grain boundary (GB) in which an extrinsic edge dislocation is absorbed. The results obtained by both discrete dislocation plasticity and quasicontinuum theory show good agreement each other. The stress field of original GB composed of intrinsic dislocation array at regular interval is short-ranged, but a long-ranged stress field is formed in the GB-dislocation interacting system (Y.Mukudai, T.Shimokawa and A.Nakatani, APCOM’07-EPMESC XI, Dec.3-6, 2007 Kyoto, JAPAN).

The discrete dislocation approach substantiated by the atomistic simulation is expected as a powerful tool for understanding the complex defect configuration which is formed by severe plastic deformation.
Residual stress distribution in severe surface deformed steel by shot peening

Masahiko Morinaga (Nagoya University), Yoshiaki Akiniwa (Nagoya University), Hideharu Nakashima (Kyushu University), Kenji Kaneko (Kyushu University), Tadakatsu Ohkubo (National Institute for Material Science), Tetsu Ichitsubo (Kyoto University), Masanori Fujinami (Chiba University), Hiroshi Numakura (Osaka Prefecture University), Hideki Araki (Osaka University), Seiichirou Ii (Sojo University)

The compressive stress distribution below the specimen surface of a nanocrystalline medium carbon steel was investigated nondestructively by using high-energy X-rays from a synchrotron radiation source. By using the monochromatic X-ray beam, the stress values at the depth of from 0.5 to 250 μm were measured by the constant penetration depth method. Measured stress corresponds to the weighted average associated with the attenuation of the X-rays in the material. The real stress distribution was estimated by using the optimization technique. The predicted stress distribution agreed very well with that measured by the conventional surface removal method.

First-principles calculations of metallic grain boundaries toward the understanding of the properties of high-density defect materials

Masanori Kohyama, Shingo Tanaka (National Institute of Advanced Industrial Science and Technology), Masato Yoshiya (Osaka University), Tokuteru Uesugi (Osaka Prefecture University)

Metallic materials formed by giant straining process contain microstructures with sub-micron grains, where the ratio of grain-boundary regions is substantial. Thus it is crucial to examine the structure and properties of grain boundaries and the interactions between dislocations and grain boundaries so as to understand the formation process and mechanical properties of the high-density defect materials. The A03(f) group has started the first-principles calculations of metallic grain boundaries for this purpose. Figure shows the iso-surfaces of the valence-charge density for the same coincidence tilt boundaries in Al and Cu. For the Al boundary, we can see peculiar charge distributions associated with reconstruction at the interface, although only spherical charges centered at atomic sites are observed in the Cu case. This should be caused by the different bonding nature between Al and Cu, which should cause different features as high-density defect materials.

Figure. Iso-surfaces of the valence-charge density in the \{122\} Σ=9 boundaries in Al (upper) and Cu (lower) (Wang, Tanaka and Kohyama, 2007). Iso-surfaces are plotted for each supercell containing two interfaces indicated by red arrows.
SPD review article selected as new hot paper

The Institute for Scientific Information has introduced the following review article as one of the most cited papers appearing in the field of Materials Science in 2006.

"Producing Bulk Ultrafine-Grained Materials by Severe Plastic Deformation"
R.Z. Valiev, Y. Estrin, Z. Horita, T.G. Langdon, M.J. Zehetbauer and Y.T. Zhu,

Prof. Zenji Horita, leader of this Giant Straining Process (GSP) program, co-authored with the other NanoSPD Steering Committee members to publish it. Prof. Ruslan Z. Valiev, chairman of the committee, commented in the Thomson Essential Science Indicators website by responding to questions such as

(1) Why do you think your paper is highly cited?,
(2) Does it describe a new discovery, methodology, or synthesis of knowledge?, with several other questions.

(see more at the website http://www.esi-topics.com/nhp/2007/july-07-RuslanZValiev.html)

Excellent tensile property of pure Fe attained by HPT

A Japanese newspaper, The Nikkan Kogyo Shimbun, reported on September 17, 2007 that the research group of Toyohashi University of Technology, Prof. Minoru Umemoto and Prof. Yoshikazu Todaka, successfully achieved high strength and high ductility of pure Fe after processing with high pressure torsion (HPT). They processed pure Fe with impurity level of 11C, <30Si, <30Mn, <20P, <3S, 300Al, <30Cr, <30Cu, <20Ti, <2B, 8N, 14O (mass ppm) for ten turns at 0.2 rpm under 5 GPa, giving the tensile strength of 1.9 GPa and the total elongation of 33 %. This report promised not only for investigating the mechanism for simultaneous enhancement of strength and ductility but also for gaining interest of industrial application.

Latest information

6th Pacific Rim International Conference for Materials (PRICM-6),
November 6-9, 2007 Jeju Island, Korea
http://www.pricm-6.org

2008 TMS Annual Meeting, including a session on Ultrafine Grained Materials, Fifth International Symposium (UFG V)
March 9-13, 2008, New Orleans, LA, USA
http://www.nanoSPD.org

Recent Developments in the processing and applications of structural metals and alloys
June 22-27 2008, Como Lake, ITALY
Contact: m.cabibbo@univpm.it

The 4th International Conference on Nanomaterials by Severe Plastic Deformation (NanoSPD4) abstract due by November 30, 2007
August 18-22, 2008, Goslar, Germany
http://www.nanospd4.org

11th International Symposium on Physics of Materials (ISPMA 11)
August 24-28, 2008, Prague, Czech Republic
http://material.karlov.mff.cuni.cz/events/ispma11

The 11th International Conference on Aluminum Alloys (ICAA11)
September 22-26, 2008, Aachen, Germany
http://www.dgm.de/icaa11

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