Award

1.Zenji Horita,	March 2012, Top Hottest article 2011 in Materials Science Engineering A, "High-pressure torsion of hafnium", Materials Science and Engineering: A, 527 (2010) 2136-2141.
2.Yoji Mine,	March 2012, Top Hottest article 2011 in Scripta Materialia, "Hydrogen trapping on lattice defects produced by high-pressure torsion in Fe-0.01 mass% C alloy", Scripta Materialia,63(2010) 552-555.
3.Hajime Kimizuka,	March 2012, Young Scientist Award, The Physical Society of Japan.
4.Yo Tomota,	May 2012, Tawara Award (The Best Year's Paper Award), The Iron and Steel Institute of Japan.
5.Zenji Horita,	February 2012, Top Cited Author 2011 in Materials Science Engineering A, "Microstructural evolution in pure aluminum processed by high-pressure torsion", Materials Science and Angineering: A, 503 (2009) 32-36. Publisher Materials Science, Elsevier.
6.Nobuhiro Tsuji,	December 2011, Meritorious Award, Kansai Branch of Japan Institute of Light Metals.
7.Yo Tomota,	November 2011, The Japan Institute of Metals Micrograph Award, The Japan Institute of Metals.
8.Yo Tomota,	November 2011, Best Poster Award, 1st Asia-Oceania Conference on Neutron Scattering.
9.Zenji Horita,	November 2011, Distinguished Service Medal of the 60th anniversary of the Japan Institute of Light Metals.
10.Masaharu Kato,	November 2011, Materia Japan Award for Education, The Japan Institute of Metals.
11.Hiromi Miura,	November 2011, The Best Paper Award, Japan Copper and Brass Association.
12.Satoshi Hata,	November 2011, Materia Japan Award for Science and Technology, The Japan Institute of Metals.
13.Yoji Miyajima,	November 2011, The Japan Institute of Metals Young Researcher Award (Microstructures), The Japan Institute of Metals.
14.Kei Ameyama,	October 2011, Best Poster Award (1st prize), Japan-China Nano-Structure Research Workshop.
15.Kei Ameyama,	Octover 2011, Excellent Poster Award (3rd prize), Japan-China Nano-Structure Research Workshop.
16.Minoru Nishida,	August 2011, First Place (Class 4 Electron Microscopy Scanning), International Metallographic Contest-2011.
17.Minoru Nishida,	August 2011, Honorable Mention (Class 3 Electron Microscopy-Transmission and Analytical), International Metallographic Contest-2011.
18.Nobuhiro Tsuji,	May 2011, Best Poster Award (Gold Medal), The 4th Int. Workshop on Materials Behavior at Micro- and Nano- Scale.
19.Yukio Takahashi,	April 2011, The Young Scientists' Prize, The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology.

Also another 13 awards.

Press

1. Yomiuri Newspaper, 29 September 2011, "Atom-specific microscopy",Yukio Takahashi.
2. Kanagawa Newspaper, 28 October 2011, "Challenges for mass production of the super high strength Mg alloys, Expectations in aerospace industries", Hiromi Miura.
3. Kagaku newspaper, 14 October 2011, "Visualization of electron density and elemental distribution in materials" , Yukio Takahashi.
4. Nikkan Kogyo newspaper, 3 October 2011, "Large field of view and high spatial resolution x-ray microscopy", Yukio Takahashi.
5. The Chemical Daily, 3 October 2011, "Realization of elemental identification in x-ray microscopy", Yukio Takahashi.

Latest information

< International Meeting >

International Workshop on Bulk Nanostructured Metals

June 26-29, 2012, Kyoto University Clock Tower Centennial Hall, Kyoto, Japan. (http://www.bnm.mtl.kyoto-u.ac.jp/2012workshop)

The workshop involves all experimental, theoretical, and simulation works on bulk nanostructured metals. Representative topics are listed below.

- Processing and Fabrication of BNMs: severe plastic deformation, powder metallurgy, mechanical alloying, electro-deposition, etc.
- Microstructures and nanostructures of BNMs
- Mechanical Properties and Deformation Mechanisms of BNMs
- Other Functional Properties of BNMs
- Phase Transformations in BNMs
- Novel Technologies for Analysis of BNMs

International Invited Speakers

Prof. Andrew Godfrey (Tsinghua University, Beijing, China), Dr. Niels Hansen (Riso-DTU, Roskilde, Denmark), Dr. Xiaoxu Huang (Riso-DTU, Roskilde, Denmark), Prof. Hyoung-Seop Kim (POSTECH, Pohang, Korea), Dr. Reinhard Pippan (Erich Schmid Institute of Materials Science, Leoben, Austria), Dr. Nairong Tao (Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China), Prof. Gerhard Wilde (University of Munster, Munster, Germany), Prof. Michael Zehetbauer (University of Vienna, Vienna, Austria), Prof. Ting Zhu(Georgia Institute of Technology) Atlanta, U.S.A.

< Domestic Meeting >

"Bulk Nanostructured Metals" Symposium in 2012 Annual Autumn Meeting of The Japan Institute of Metals September 17-19, 2012, Matsuyama, Japan
http://jim.or.jp/e/An-Me/2012_Fall-index.html

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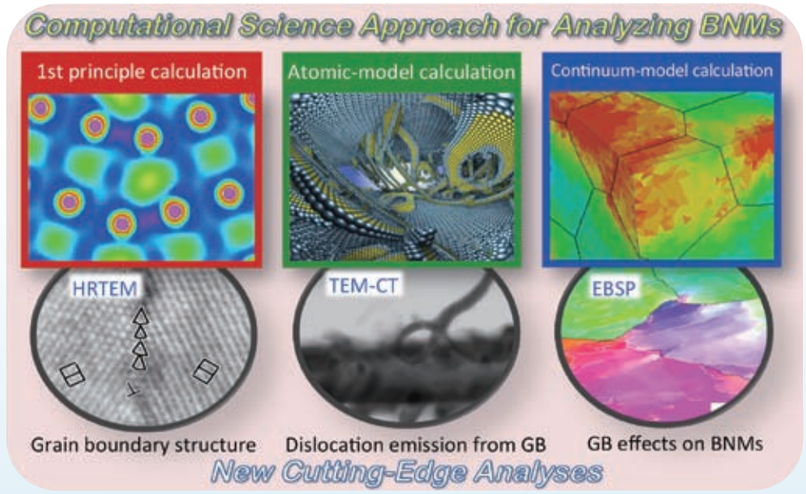
BNM June 2012 NEWS LETTER No.2
http://www.bnm.mtl.kyoto-u.ac.jp/index_e.html

Bulk Nanostructured Metals

Project Leader : Nobuhiro Tsuji (Kyoto University)

Computational Science Approach for Analyzing Bulk Nanostructured Metals

"Bulk Nanostructured Metals (BNM)" are the bulky polycrystalline materials composed of matrix grains or phases having sizes smaller than 1 μm; hence BNMs are considered as the materials "full of grain boundaries". Because BNMs show unique mechanical properties, it is expected that the BNMs can give a big impact on our society. This project aims to systematically clarify the relationship between the peculiar properties of BNMs and their structures through close collaboration of researchers in various fields. This project is mainly organized into three groups: A01(Structure Design), A02(Processing) and A03 (Mechanical Properties), and each group consists of two sub-groups: one is focusing on experimental studies (A01a, A02c and A03e), the other on theoretical and simulation studies (A01b, A02d and A03f). This news letter introduces the computational science approach for analyzing the BNMs using the 1st principal, atomic-model and continuum-model calculations *with the collaboration of experimental and new cutting-edge analytical studies*.

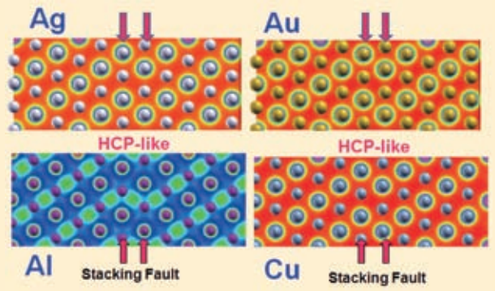


1st principle

Development of First-Principles Local-Energy and Local-Stress Schemes and Applications to Metallic Grain Boundaries, Stacking faults and Defects toward the Materials Design of Bulk Nanostructured Metals

Masanori Kohyama and Shingo Tanaka (National Institute of Advanced Industrial Science and Technology, A01b)

In usual first-principles methods based on density-functional theory, total energy and stress are given as the integral or average throughout the supercell. If such quantities were given in each local region, defective systems could be deeply analyzed. Local energy-density and stress-density schemes were proposed previously, while practical applications have not yet been performed, due to the difficulty in the gauge-dependent problem. Recently, the practical way to settle the gauge-dependent problem was proposed [1], and the energy and stress densities have been formulated in the projector augmented wave (PAW) method for the first time. In the present research, we develop practical computational techniques to calculate local energy and local stress via the Bader or Voronoi integration of energy and stress densities, according to the proposed strategy [1]. We apply the developed techniques to metallic grain boundaries, stacking faults and defects with and without impurities, which dominate the stability and mechanical properties of bulk nanostructured metals. Figure shows the valence charge distribution at the intrinsic stacking faults in Al, Cu, Ag and Au. The calculated stacking-fault energy has the order as Al>>Cu>Au>Ag, of which the origin can be effectively analyzed by the local energy analysis. *The analysis of the relation among Cu, Ag and Au can well explain the experimental results of HPT (High-Pressure Torsion) samples by the group of Prof. Horita, A02c [2].*



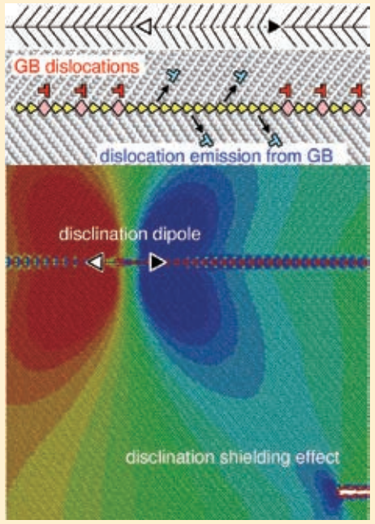
[1] Y. Shiihara, M. Kohyama and S. Ishibashi, "*Ab initio* local stress and its application to Al (111) surfaces", *Phys. Rev. B*, **81** (2010), 075441 (1-11).
[2] H. Matsunaga and Z. Horita, "Softening and Microstructural Coarsening without Twin Formation in FCC Metals with Low Stacking Fault Energy after Processing by High-Pressure Torsion", *Mater. Trans.*, **50** (2009) 1633-1637.

Atomic model

Disclination Shielding Effect on the Fracture Toughness of Bulk Nanostructured Metals by Atomic Simulation

Tomotsugu Shimokawa (Kanazawa University, A03f) and Masaki Tanaka (Kyushu University, A03e)

It has been reported that bulk nanostructured metal shows improved fracture toughness at low temperatures as compared to coarse-grained metal. *Based on the dislocation shielding theory and experimental results about dislocation mobility reported by Prof. Tanaka in the BNM project group A03e [1], a stronger crack tip shielding effect is required without reducing the plastic deformation ability around the crack tip*. In order to investigate the roles of grain boundaries in improving the fracture toughness of bulk nanostructured metals, the interactions among crack tips, dislocations, and grain boundaries are investigated with aluminum bicrystal models using molecular dynamics simulations. Based on the results of our atomic simulations [2], the role of grain boundaries as dislocation sources should be essential to elucidate fracture phenomena in bulk nanostructured metals. A proposed mechanism to express the improved fracture toughness in ultrafine-grained metals is the disclination shielding effect on the crack tip mechanical field. Disclination shielding can be activated when a transition of dislocation sources from crack tips to grain boundaries and a transformation of the grain boundary structure into a neighboring energetically stable boundary by emitting dislocations from the grain boundary occurs. The disclination shielding effect becomes pronounced as dislocations are continuously emitted from the grain boundary without dislocation emissions from crack tips.



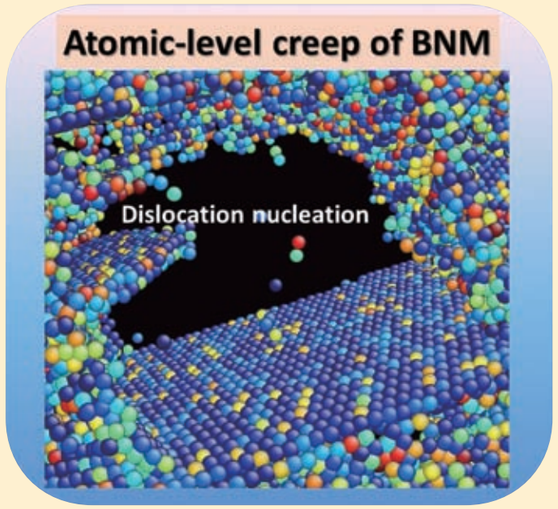
[1] M. Tanaka, K. Higashida, T. Shimokawa and T. Morikawa, “Brittle-Ductile Transition in Low Carbon Steel Deformed by the Accumulative Roll Bonding Process”, *Mater. Trans.*, **50**(2009), 56-63.
[2] T. Shimokawa, M. Tanaka, K. Kinoshita and K. Higashida, “Roles of Grain Boundaries in Improving Fracture Toughness of Ultrafine-Grained Metals”, *Phys. Rev. B*, **83** (2011), 214113(1-13).

Atomic model

Atomistic Simulation of Creep in Bulk Nanostructured Metals

Yunjiang Wang and Shigenobu Ogata (Osaka University, A01b)

The mechanical and electronic properties of materials have been significantly advanced by reducing the characteristic sample size or grain size to nanoscale regime. However, the enhanced creep of nanostructured materials limits their utilities at mediate and high temperature of service. Thus, understanding creep in BNM with atomistic details can be valuable not only for scientific purpose but also for engineering information about improving the stability and lifetime of these advanced materials. Atomistic level simulations provide new knowledge on creep of BNM [1,2]: (1) Competing thermal activated, rate-controlling diffusive and displacive deformations, namely, grain boundary (GB) diffusion, GB sliding and migration, and dislocation nucleation from GBs cooperatively dominate creep in BNM. (2) *In collaboration with Prof. M. Kato in the BNM project group A03e, we find strong entropic effect on creep of BNM, which originates from anharmonic effect during thermal activation*. (3) Size effect arises in creep of BNM, in contrast with its conventional coarse-grained counterpart. These findings widely broaden our understanding on creep in BNM.



[1] Y. J. Wang, A. Ishii and S. Ogata, "Transition of creep mechanism in nanocrystalline metals", *Phys. Rev. B*, **84** (2011), 224102(1-7).
[2] Y. J. Wang, A. Ishii and S. Ogata, "Grain Size Dependence of Creep in Nanocrystalline Copper by Molecular Dynamics", *Mater. Trans.*, **53** (2012), 156-160.

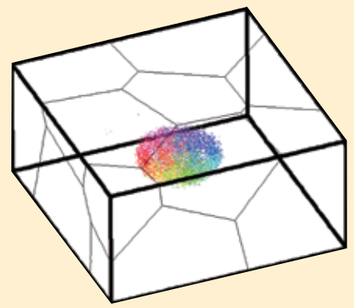
Continuum model

Multiscale Modeling and Simulation Considering Effects of Grain boundary on Bulk Nanostructured Metals

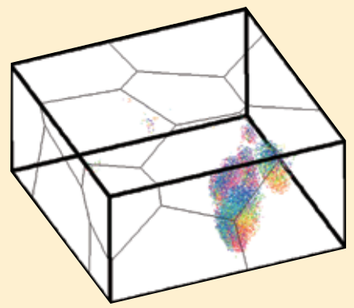
Yoshiteru Aoyagi (Tohoku University, A03f)

Whereas bulk nanostructured metals produced by severe plastic deformation express remarkably peculiar behavior in both material and mechanical aspects, its mechanism has been clarified by neither experimental nor computational approaches. In this study, a multiscale crystal plasticity model considering an effect of grain boundary is developed [1]. In order to express release of dislocation from grain boundaries, information of misorientation is introduced into a hardening law of crystal plasticity. *The presented model is improved on basis of experimental and numerical results of deferent scale obtained by the other research group in this project, A03e and A03f [2].* Carrying out FE simulation for FCC polycrystal, the stress-strain responses such as increase of yield stress due to existence of grain boundary are reproduced. This model can express the dislocation behavior from mesoscopic viewpoint.

[1] Y. Aoyagi, T. Shimokawa, K. Shizawa and Y. Kaji, "Simulation on Nanostructured Metals Based on Multiscale Crystal Plasticity Considering Effect of Grain Boundary", *Materials Science Forum*, **706-709**(2012), 1751-1756.
[2] N. Kamikawa, X. Huang, N. Tsuji, N. Hansen, "Strengthening mechanisms in nanostructured high-purity aluminium deformed to high strain and annealed", *Acta Materialia*, **57** (2009), 4198-4208.



GN dislocation released from dislocation source



GN dislocation released from grain boundary

Continuum model

Strain Variation on Rolling Condition in Accumulative Roll-bonding (ARB) by Finite Element Simulation

Tadanobu Inoue (National Institute for Materials Science, A02d), Nobuhiro Tsuji (Kyoto University, A01a)

In bulk nanostructured metals, since the microstructural evolution of plastically deformed materials is directly related to the magnitude of plastic deformation, the understanding of the phenomenon associated with the strain development is very important. For the ARB process, the microstructure and texture in a sheet processed by one ARB cycle without lubricant dramatically change depending on the thickness location of the sheet. In a rolling process, including ARB, these changes are caused by the shear strain imposed by friction between rolls and sheet, and roll bite geometry, L_d/t_d (see Figure) [1]. *A quantitative relation among the strains, friction, and roll bite geometry obtained from numerical simulations would provide useful guidelines for studying the correlation between microstructures and strain in ARB process as well as the microstructure design in a rolled sheet [2].*

[1]T. Inoue, “Finite element analysis”, Editor: David Moratal, SCIYO, Croatia, (2010), pp.589-610.
[2] T. Inoue and N. Tsuji, “Quantification of strain in accumulative roll-bonding under unlubricated condition by finite element analysis”, *Comp. Mater. Sci.*, **46** (2009), 261-266.