03-4 IUTAM Symposium on Mesoscopic Dynamics of Fracture Process and Materials Strength Osaka, Japan, 6 - 11 July 2003

a) Scientific Committee

H. Kitagawa(Japan, Co-Chairman), Y. Shibutani(Japan, Co-Chairman), P. Gumbsch(Germany), L.P.Kubin(France), A. Needleman(USA), S. Schmauder(Germany), S. Yip(USA), B. Freund (USA, IUTAM Representative)

b) Short summary of scientific progress achieved

It is essential to tackle dynamical structural change in mesoscopic scale to evaluate the materials strength and damage due to fracture. To take a concrete action toward this viewpoint is the main purpose of the Symposium, a ground of which is built on the following observation.

Deformation of materials involves internal dissipation more or less. Energy dissipation proceeds usually, accompanying with evolution of ordered internal mechanism through which so-called ‘dissipative structure’ works. This structure behaves dynamically in nature and is set up in a state far from equilibrium. Although the ordered structure varies in scale and phase (pattern) corresponding to the intensity of energy dissipation required, overall deformation still continues as long as it operates as a whole. Appearance of a new phase issues necessarily from an embryo and diffuses or propagates into surrounding. But if it fails to get a certain territory of influence, being unable to overleap the adjoining energy barrier, the energy to be dissipated accumulates locally and the material falls into failure process. This is a general situation around the site in the materials to bear the load.

The points at issue presented through the Symposium were just around the subjects in relation to the above understanding, which include the justification and/or appropriateness of such an understanding for the fracture process, actual methodology to extract the mesoscopic dynamics into the analysis, concrete trials to approach to the reality of simultaneous interaction

between microscopic events and macroscopic phenomena and successful results to estimate the material strength and to describe the actuality of fracture process, and others.

The progress achieved is productive and manifold, which may be seen from the titles of presented papers shown in the scientific program. A couple of concrete topics to impress the participants are: For analysis of fracture process and estimation of the materials strength to target at dynamics evolution of the inner structure, hierarchical modeling is essential to catch heterogeneity in mesoscopic scale through which dynamics of atomistic structure and macroscopic mechanical field interact simultaneously. Approach based on continuum mechanics may be still powerful, but simple material model becomes undependable because non-locality due to the inner mesoscale structure is excluded. Moreover, the traditional approach based on a mathematical or conceptual constitutive formalism itself might not be a strong tool, because expression of the material properties, i.e. formulation of the constitutive equation, is not treated as a problem of the mechanics. As a result, the continuum approach should be sophisticated towards the following ways: the material parameters are not given a priori, but they are evaluated by an evolutional way from microscopic structural dynamics, and mesoscopic material heterogeneity should be treated as an inner boundary value problem.

“Computer changes way of thinking about the nature”, this is the actual impression striking the participants of the Symposium.

c) Countries represented and number of participants

The meeting attracted 66 participants from 8 countries: Denmark(1), France(6), Germany(3), Japan(37), Korea(2), Russia(2), United Kingdom(2), USA(8)

d) Publication of Proceedings of the Symposium

The Proceedings of the Symposium, edited by H. Kitagawa and Y. Shibutani, will be published by Kluwer Academic

Publishers, as a monograph in the Series of Solid Mechanics and Its Application.

e) Financial supports

The Symposium was sponsored by the following organizations:

- International Union of Theoretical and Applied Mechanics(IUTAM)
- Graduate School of Engineering, Osaka University
- The Japan Society of Mechanical Engineers(JSME)
- The Society of Materials Science, Japan(LSMS)
- Handai Frontier Research Center(FRC)
- Japan Society for Promotion of Science(JSPS)

We are grateful to our sponsors for their contributions to the success of the symposium

f) Scientific program

Session 1: DDD, Dislocation Patterning

W. Cai, V. V. Bulatov, T. Pierce, M. Hiratani, M. Rhee and M. Bartelt, *Dislocation Patterning and Plasticity*

Y. Kaneko and S. Hashimoto, *Nondestructive Observation of Dislocation Structure Formed at Fatigued Copper and Stainless Steel Crystals*

D. Weygand, *Plasticity in Small Samples: A Discrete Dislocation Dynamics Description*

R. Madec, *A Dislocation Dynamics Study of Some Constitutive Parameters for Plastic Flow*

Session 2: MD, DDD, Crystal Plasticity

E. Bitzek, D. Weygand and **P. Gumbsch**, *Atomistic and DDD Studies of Inertial Effects on the Dynamics of Dislocations*

K. Yashiro, Y. Tabata and Y.Tomita, *Molecular Dynamics Study on the Characteristics of Edge and Screw Dislocations in Gamma/Gamma-Prime Microstructure in Ni-based Superalloy*

L.P. Kubin, *Multiscale Modeling of fcc Single Crystal Plasticity*

V. S. Deshpande, **A. Needleman** and E. Van der Giessen, *Discrete Dislocation Modeling of Fatigue Crack Growth in Single Crystals*

Y. Aoyagi and **K. Shizawa**, *A Crystal Plasticity Analysis for Accumulations of Geometrically Necessary Dislocations and Dipoles around Shear Band*
T. Ohashi, *A New Model of Scale Dependent Crystal Plasticity Analysis*

Session 3: MD, Amorphous, Silicon, Fracture
K. Nakatani, Y. Sugiyama and H. Kitagawa, *Molecular Dynamics Study on Mechanisms of Deformation and Fracture near a Crack Tip in Amorphous Metal*
S. Izumi, S. Hara, T. Kumagai and S. Sakai, *Elastic Properties of the Surfaces and Interfaces of Crystal and Amorphous Silicon*
S. Brochard, J. Godet, L. Pizzagalli, P. Beauchamp and J. Grilhe, *Atomistic Simulation of Dislocation Generation at Surface Defects in Metals and Silicon*
P. Pirouz, *On the Plasticity and Fracture of Semiconductors*
K. Higashida and M. Tanaka, *HVEM/AFM Studies on Crack Tip Plasticity in Si Crystals*

Session 4: MD, Dislocation, Obstacle, Indentation
D. Rodney, *Atomic and Mesoscopic Modeling of Irradiation Hardening in FCC Crystals*
D.J. Bacon, Yu. N. Osetsky, Z. Rong and K. Tapassa, *Dynamics of an Edge Dislocation Glide in the Presence of Substitutional Solute Atoms and Glissile Interstitial Clusters*
H. M. Zbib, Mu'tasem, A. Shehadeh, Tomas. D. de la Rubia and V. Bulatov, *Modeling the Dynamic Behavior of FCC Single Crystals under Shock Loading: Dislocation Dynamic Plasticity Analysis*
Yu. N. Osetsky and D. J. Bacon, *Atomic-Level Interaction of an Edge Dislocation with Localized Obstacles in Fcc and Bcc Metals*
K. J. Van Vliet, J. Li, T. Zhu, S. Suresh and S. Yip, *Understanding Defect Nucleation through Nanoscale Experiments and Computations*
T. Tsuru and **Y. Shibutani**, *Dislocation Emission and Prismatic Dislocation Loop Formation of Single Crystalline Aluminum under Nanoindentation*

Session 5: Multiscale Modeling

S.Yip, *Multiscale Modeling of Materials Strength and Deformation*

S. Schmauder, U. Weber, P. Binkele and P. Kizler, *Parameter Link as an Approach to Hierarchical Modelling of Toughness Decrease of Steels*

B. Devincre, *Modelling Plasticity at Mesoscale with Dislocation Dynamics and Finite Elements Coupling*

Y. Tomita and M. Uchida, *Computational Evaluation of Micro- to Macroscopic Deformation Behavior of Amorphous Polymer with Slightly Heterogeneous Distribution of Molecular Chains*

Y. Higa, H. Kitagawa and Y. Tomita, *Computational Evaluation of Micro- to Macroscopic Deformation Behavior of Amorphous Polymer with Slightly Heterogeneous Distribution of Molecular Chains*

Session 6: Crack, DB Transition, Transformation

I. L. Maksimov, *Critical Behavior near the Crack/Dislocation Depinning Threshold: Critical Indices and Landau-type Expansion*

S. V. Dmitriev, N. Yoshikawa and A. A. Vasiliev, *Domain wall and dislocation dynamics in media with microscopic rotations*

J. W. Kysar, *Dependence of Ductile and Brittle Response on Initial Energy Dissipation Mechanism at Crack Tip*

K. Kishimoto, *A Cohesive Zone Model and Interfacial Crack Problems*

S. Kubo and M. Misaki, *Molecular Dynamic Simulation of Influence of Crystallographic Orientation and Grain Boundary on Near-Threshold Fatigue Crack Growth in Iron*

Y. Nakasone, S. Kasumi and Y. Iwasaki, *Plasticity-Induced Martensitic Transformation around Semi-elliptical Surface Cracks in Fatigue of an Austenitic Stainless Steel*

Session 7: Nano-crystal, Poly-crystal

Y.-S. Kim, C.-Il Kim and S.-S. Lee, *An atomistic simulation of AFM-based nano lithography process for nano patterning*

K. Saitoh, S. Nagase, H. Kitagawa and N. Shinke, *Molecular Dynamics Study on Morphology and Strength of Copper Atomic-cluster-assembled Structure*

J. Schiotz, *The Strength of Nanocrystalline Metals: An Optimal Grain Size*
A. Nakatani, T. Shimokawa, R. Matsumoto and H. Kitagawa, *An Atomistic Study of Ideal Strength of Polycrystalline Metals*
T. Hasebe, *Continuum Description of Inhomogeneously Deforming Polycrystalline Aggregates based on Field Theory*

Session 8: Ab-initio Calculation, Mutiscale Modeling
Y. Umeno and T. Kitamura, *Study on Strength of Microscopic Material by Simulations with Atom and Electron Models*
S. Ogata, J. Li, Y. Shibutani and S. Yip, *Ab initio Study of Ideal Shear Strength*
C. Domain and A. Legris, *Ab initio Atomic-scale Simulation Investigation of the Plasticity in Zirconium and Titanium – Influence of Hydrogen*
M. Kohyama, S. Tanaka and R. Yang, *Computational Study of the Mechanical Properties of Alumina-Copper Interfaces: Ab initio Calculations and Combination with Mesoscopic Simulations*
S. Ogata, *A Hybrid Electronic-Density-Functional/Molecular-Dynamics Simulation Scheme for Multiscale Simulation of Materials on Parallel Computers*

Report composed by Hiroshi Kitagawa