NU-NIMS Center for Materials Innovation

Joint Materials Genome Workshop Report

Northwestern University, Evanston, IL

March 25-26, 2014

Co-organized by:

National Institute of Materials Science, Japan

Northwestern University, USA

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Section 1 Acknowledgements

As Co-Directors of the NU-NIMS Center for Materials Innovation (NU-NIMS-CMI), we are continuously in awe of the remarkable NU and NIMS researchers who make this Center possible. We are genuinely grateful for their enthusiasm for collaboration and commitment to traveling to our respective countries to pursue the exchange of information, goals, and understandings. Despite busy schedules and numerous commitments, everyone participated with the hope that, together, we could lead the world in solving challenges in energy, environment, and security.

The Center is co-sponsored by the International Materials Institute for Solar Energy and Environment, and we are thankful for their funding and singular commitment to the Center's mission and efforts. The National Science Foundation also sponsors the Center through the Materials Research Institute.

We also thank Dr. Koichi Tsuchiya (NIMS) and Prof. G.B. Olson (NU) for their leadership and organizing the workshop.

Being a part of this Center and collaborating at our highly-effective workshops point toward a brighter future in which every country participates in joint materials science innovation for the well-being of future generations. We are excited to see what powerful and creative solutions we can come up with together through NU and NIMS!

Sincerely,

Co-Directors of the NU-NIMS-CMI:

R.P.H. Chang
Professor, Materials Science and Engineering, Northwestern University
Director, International Materials Institute for Solar Energy and Environment

Dr. Yoshio Aoki
Director, External Collaboration Division, National Institute for Materials Science

Section 2 Executive Summary

This is the third in a series of NU-NIMS workshops, which was held in Evanston, IL. The inaugural workshop for the NU-NIMS Center for Materials Innovation took place in Evanston, IL on September 5, 2012, while the second workshop was held at NIMS, Tsukuba on March 1, 2013. On March 26, 2014, faculty members from Northwestern participated in a one-day intensive discussion with NIMS researchers at Northwestern on the Evanston campus. A large array of research topics was covered, ranging from hydrogen embrittlement, titanium alloys, and cobalt alloys, to high temperature materials, microstructure modeling, and finite element analysis. Parallel discussion groups were held throughout the day and many good ideas were generated for potential collaborations in terms of exchange visits and the use of shared facilities.

The mission and goal of these workshops are to identify the unique projects that will benefit both Japan and the U.S. Through joint publications and exciting preliminary findings, opportunities will be identified for joint research funding of small and large programs. Researchers, both at NIMS and Northwestern, are encouraged to continue with the dialogues and start to implement some of the collaboration plans.

Section 3 Materials Genome Workshop Highlights

The third meeting and workshop of the NU-NIMS Center for Materials Innovation was held on March 26, 2014 at Northwestern University in Evanston, IL. The goal of this one day workshop was to build on the first and second meetings' discussions from September 5, 2012 and March 1, 2013 matching researchers for collaboration work.

This year's focus is on materials related to infrastructure, transportation, and construction in order to minimize energy consumption and protect the environment. The theme for this meeting was the Materials Genome Workshop. During this time, we strived to understand from basic theory to simulation in order to design and optimize the time for searching new materials, processing, and quickly performing iterative design to reach the final desired material. This requires theory, simulation, modeling, database, experiments, and materials characterization, all performed in a cross-disciplinary and effective way.

The one-day workshop consisted of various topics from researchers in the following areas of the agenda:

- Advanced alloys
- New characterization tools
- Computational material science
- Novel processing

Section 4 Workshop Program

Wednesday, March 26, 2014 **Ford Design Center**
ITW Room

8:30 AM	Registration (Coffee & Pastry)	
	A. Opening	
8:50	Welcome	Prof. G.B. Olson, Northwestern Dr. Y. Aoki, NIMS
	B. Advanced Alloys	
9:00	Strength-Ductility Balancing by Twinning Optimization in Austenitic Steel	Prof. K. Tsuzaki, Kyushu U
9:20	Hydrogen Embrittlement of High Strength Steels	Dr. Eiji Akiyama, NIMS
9:40	Improvement of Mechanical Properties of Beta Ti Alloys Using Heterogeneity	Dr. Satoshi Emura, NIMS
10:00	Cobalt Alloys	Prof. D. Dunand, NU
10:20	***BREAK***	
10:40	Oxidation Resistant Coatings for High Temperature Structural Materials	Dr. Hideyuki Murakami, NIMS
11:00	Elements Strategy Initiative	Prof. Nobuhiro Tsuji, Kyoto U
	C. New Characterization Tools	
11:20	Introduction of Facilities and Research Activities at the NIMS Contract Beamline BL15XU of SPring-8	Dr. Osami Sakata, NIMS
11:40	APS Research	Prof. M. Bedzyk, NU
12:00 PM	***LUNCH***	**Allen Center**
	D. Computational Materials Science	
1:30	Simulation of Electronic Structures and Stability of Body-centered Cubic Ti-Mo Alloys by Special Quasirandom Structures	Dr. Ryoji Sahara, NIMS

1:50	FLAPW Applications	Dr. O. Kontsevoi & Prof. A.J. Freeman, NU
2:10	Mathematical Homogenization of Discrete Models with Rotational Degrees of Freedom	Dr. Roozbeh Rezkhani & Prof. Gianluca Cusatis, NU
2:30	Homogenization Analysis Based on Finite Element Method at Continuum Scale	Dr. Ikumu Watanabe, NIMS
2:50	Microstructure Modeling	Prof. P.W. Voorhees, NU
3:10	***BREAK***	

E. Novel Processing

3:30	Effect of Nitrogen Flow Rate on Mechanical Properties of Metallic Coatings by Warm Spray Deposition	Dr. Makoto Watanabe, NIMS
3:50	Nanotribology	Dr. Y. Liao & Prof. L. Marks, NU
4:10	Characterization of Microstructure and Local Mechanical Properties in Weldments	Dr. Satoru Kobayashi, NIMS
4:30	Ultrafine Grain Formation by in situ Precipitation During SPD in Mg Alloy	Dr. Koichi Tsuchiya, NIMS
4:50	Additive Manufacturing	Prof. G.B. Olson, NU

5:15 ***ADJOURN***

Section 5 Strategic Planning Discussion

A strategic planning discussion took place on March 25th, 2014. Attendees convened to discuss a broader collaboration between the US and Japan in the area of materials genome research that integrates theory, modeling, simulation, experiments, database, design, and fabrication. The NU-NIMS Center for Materials Innovation (NU-NIMS-CMI) will work with the Center for Hierarchical Materials Design (CHiMaD) to launch the next Japan-US workshop to expand the scope of this important research area, with applications for future materials related to structure, transportation, and energy. The collaboration is envisioned to expand to include larger cooperation from both sides.

Photo names, titles, and affiliations from left to right:

Dr. Yibin Xu (Group Leader, Materials Database Group, NIMS)

Dr. Akitsu Shigetou (Senior Researcher, Interconnection Design Group, NIMS)

Dr. Yoshio Aoki (Division Director, External Collaboration Division, NIMS; Co-Director of NU-NIMS-CMI)

Prof. Peter Voorhees (Professor, Materials Science and Engineering, Northwestern University; Director of CHiMaD)

Prof. R.P.H. Chang (Professor, Materials Science and Engineering, Northwestern University; Co-Director of NU-NIMS-CMI)

Dr. Takuya Kadohira (Senior Engineer, Research and Analysis Office, NIMS)

Mr. Takefumi Notomi (Group Head, Academic Collaboration Office, NIMS)

Section 6 Photographs