CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

TRIP REPORT

SUBJECT: 2005 Solid-Solid Phase Transformations in Inorganic Materials Conference (AI 06002.322.507)

DATE/PLACE: May 29–June 3, 2005
Phoenix, Arizona

AUTHOR: Y.-M. Pan

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AUTHOR:	Y.-M. Pan
PERSONS PRESENT:	Y.-M. Pan, Center for Nuclear Waste Regulatory Analyses (CNWRA) and approximately 300 participants from 19 countries attended the conference

BACKGROUND AND PURPOSE OF TRIP:

The purpose of this trip was to attend and present a poster at the International Conference on Solid-Solid Phase Transformations in Inorganic Materials. The present conference is the fifth in a series that began in 1981 at Carnegie Mellon University. The main goals of this conference are to discuss the most current developments in understanding fundamental aspects of solid-to-solid phase transformations in inorganic materials and to present critical comparisons between theory and experiment.

SUMMARY OF PERTINENT POINTS:

The 2005 Solid-Solid Phase Transformations in Inorganic Materials Conference included presentations on (i) fundamentals of phase transformations, (ii) diffusional transformations, (iii) displacive transformations, (iv) computer approaches to simulation of phase transformations, (v) experimental approaches to the study of phase transformations, and (vi) phase transformations in novel systems or special materials. Emphasis was placed on inorganic materials, including ceramic, metallic, and mineral systems. About 350 papers were presented in oral and poster sessions. Y.-M. Pan made a poster presentation of the paper co-authored by D. Dunn titled Modeling Phase Transformations of Ni-Cr-Mo Alloys. The paper discussed results of our recent computer simulations on the thermodynamic and kinetic modeling of phase transformations and solidification reactions in nickel-base alloys as influenced by alloy compositional variation.

The conference provided excellent opportunities to keep up with the new experimental and computational techniques applicable to the understanding of solid-to-solid phase transformations and to discuss our work with scientists from many countries. A series of invited papers were presented at the conference by well-known international speakers selected from various disciplines of chemistry, physics, and mathematics, as well as from materials science. A number of pertinent papers are summarized in this report.

In the area of computer approaches to simulation of phase transformations, T. Mohri (Hakkaido University, Japan) discussed first-principle calculation of ordering phase transition. Mohri used a combination of electronic structure total energy calculations with statistical mechanics

methods as a theoretical tool to perform first-principle study on the transition dynamics and kinetics of iron-base alloys. Effective interaction energies were obtained by employing a full-potential linear augmented planewave theory followed by a cluster expansion method. The homogeneous free energy density was then described within the framework of a cluster variation method. Mohri described the application of the tool to the analysis of multi-scale aspects of ordering dynamics, including the atomistic ordering, wetting, and coarsening of anti-phase boundary.

A. Walle (Northwestern University) made a presentation on automated computational tools for *ab initio* alloy thermodynamics. Walle described how the thermodynamic properties of alloys can be calculated from first principles using the Alloy Theoretical Automated Toolkit, a software package aimed at providing thermodynamic data for multicomponent alloys. Recent additions to the toolkit included the calculation of electronic and vibrational entropies, the computation of free energies in multicomponent systems, and interfaces with various first-principle computer codes. Walle also illustrated these capabilities with examples of applications to Cu-, Ni-, and Ti-base alloy systems.

J. Morral (Ohio State University) compared DICTRA, a computer code for diffusion-controlled phase transformations, and phase field simulations for predicting microstructural changes due to interdiffusion. Finite difference simulations with DICTRA can provide both concentration profiles and diffusion paths in less than an hour, but they cannot predict precipitate morphology or consider the effect of morphology on interdiffusion. Phase field simulations, on the other hand, do take into account microstructure morphology and are flexible in boundary conditions, but they have limitations in terms of computer time needed for two- and three-dimensional simulations and their ability to predict diffusion paths. Decision steps in selecting appropriate simulation tools were discussed according to the associated advantages and limitations.

In the area of experimental studies of phase transformation phenomena, E. Conforto (University of La Rochelle, France) discussed the transformation paths of titanium into several hydride phases and the role of crystallographic relationships. Conforto described in detail a transmission electron microscopy study at the surface of an acid-etched titanium substrate designed for implant and prosthesis applications. Four different orientation relationships were found between the two types of hydride (face-centered-cubic TiH_{2-x} and tetragonal TiH) and the hexagonal close-packed Ti matrix, depending on the interface plane in which the first hydride was formed. This analysis allows the determination of transformation paths to transform titanium into the two titanium hydrides.

J. Lee (Michigan Technological University) made an interesting presentation on cyclical phase transformations taking place during mechanical alloying, ion beam irradiation, and plastic deformation. Thermodynamic and kinetic aspects of cyclical phase transformations were discussed, followed by the modeling results. In the case of an internally driven system, iron nitride (Fe_4N) in α-iron, oscillatory microstructural evolution was observed, suggesting a cyclical process of precipitation and dissolution. The driving force for the cyclical behavior was attributed to the elastic strain energy associated with nitride formation.

There were two invited papers addressing fundamental aspects of phase transformations. J. Cahn (National Institute of Standard & Technology) discussed the atomic motion of solid-solid interfaces and grain boundaries by a shear stress through coupling and postulated that almost any motion of an interface can produce a coupled tangential translation. With this

postulation, several phenomena associated with grain boundary mechanics and motion can be satisfactorily explained. M. Hillert (Royal Institute of Technology, Sweden) made a tutorial presentation on treatments of deviation from local equilibrium at migrating interfaces, in which approaches based on the chemical driving forces acting on the interface were illustrated using molar Gibbs energy diagrams.

IMPRESSIONS/CONCLUSIONS

The 2005 Solid-Solid Phase Transformations in Inorganic Materials Conference was mostly attended by scientists from worldwide academic institutions and research laboratories. The participation at the conference was an excellent avenue to present the metallurgical stability modeling work conducted for the U.S. Nuclear Regulatory Commission at CNWRA. Attending this conference also promoted international interactions and provided the opportunity to keep the most current developments in phase transformations.

PROBLEMS ENCOUNTERED:

None.

PENDING ACTIONS:

None.

RECOMMENDATIONS:

Future participation at the Solid-Solid Phase Transformations in Inorganic Materials conferences is recommended.

SIGNATURE:

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6/16/2005
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