

PROGRAM

Second International Alloy Conference (IAC-2) *An Interdisciplinary Approach to the Science of Alloys in Metals, Minerals and Other Materials Systems*

**August 8-13, 1999
Davos, Switzerland**

**Conference Co-Chairs:
A. Gonis, A. Meike, K. Rajan and P.E.A. Turchi
Lawrence Livermore National Laboratory**



19990920 027

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REPORT DOCUMENTATION PAGE

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OMB No. 0704-0188

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1. REPORT DATE (DD-MM-YYYY) 15-09-99		2. REPORT DATE		3. DATES COVERED (From - To) 01-07-99 to 03-06-00	
4. TITLE AND SUBTITLE 2nd International Alloy Conference: An Interdisciplinary Approach to the Science of Alloys in Metal, Mineral and Other Materials Systems				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER N00014-99-1-0895	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) K. Rajan A. Gonis P. Turchi A. Meike				5d. PROJECT NUMBER 99-BS	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) United Engineering Foundation Inc. 3 Park Avenue 27th floor New York, NY 10016-5902				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) United Engineering Foundation Inc. 3 Park Avenue 27th floor New York, NY 10016-5902				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSORING/MONITORING AGENCY REPORT NUMBER	
12. DISTRIBUTION AVAILABILITY STATEMENT DISTRIBUTION STATEMENT A Approved for Public Release Distribution Unlimited					
13. SUPPLEMENTARY NOTES There will be no proceedings for this conference					
14. ABSTRACT This is a second Triennial Conference on the physical, chemical, and mechanical properties of materials, interpreted to mean simple and complex inorganic solids, i.e., metals, semiconductors, and mineral of technological and environmental significance					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			19b. TELEPHONE NUMBER (Include area code)
			18	52	Charles V. Freiman 212-591-7943

**We wish to thank the following organizations
for their financial support of the conference:**

Office of Naval Research

Lawrence Livermore National Laboratories

TMS

Sunday, August 8, 1999

5:00 pm - 7:00 pm

Registration

7:00 pm - 9:00 pm

Dinner

9:00 pm - 10:00 pm

Opening Reception

All meals will be at the Cresta Sun Hotel.

All Technical Sessions will be at the Congress Center.

Monday, August 9, 1999

7:00 am - 8:30 am

Breakfast

8:30 am - 8:45 am

Welcome and Introductions

Tony Gonis, Conference Co-Chair

Norm Stoloff, UEF Technical Liaison

Barbara Hickernell, Conferences Director, UEF

Session IA: Thermodynamics of Alloys: Ordering

Chairperson: A. Meike

8:45 am - 9:25 am

E. K. H. Salje

Ordering mechanisms in minerals

9:25 am - 9:45 am

H. Lang

Ordering kinetics in B₂-FeAl

9:45 am - 10:05 am

V. Vaks

**Kinetic features of non-simplest alloy orderings:
DO₃, L₁₂, and L₁₀ type orderings**

10:05 am - 10:25 am

M. Spanl

**Short-range ordering kinetics and microstructural
development during post-deformation annealing**

10:25 am - 10:55 am

Coffee Break

Session IA: Thermodynamics of Alloys: Ordering

Chairperson: K. Masuda-Jindo

10:55 am - 11:35 am

F. Schmid

**Order and disorder phenomena at surfaces of
binary alloys**

11:35 am - 11:55 am

R. V. Chepulskey

**Analytical description of the short-range order in
alloys with many-body atomic interactions**

11:55 am - 12:15 pm

B. Wuensch

**Changes in the atomic coordinates and state of
anion and cation order induced by alloying in
Y₂[M(2)YM(1)_{1-γ}]₂O₇ solid solution systems**

12:15 pm - 12:35 pm

S. I. Simak

**Ordering in Cu₂/NiZn: a first-principles Monte-
Carlo study**

Monday, August 9, 1999 (continued)

12:45 pm - 2:00 pm	Lunch
2:00 pm - 4:45 pm	<i>Ad hoc</i> sessions and/or free time
4:45 pm	Coffee Service

Session IB: Thermodynamics of Alloys: Kinetics and diffusion

Chairperson: G. Grimvall

5:00 pm - 5:40 pm	W. E. Glassley Using arrested solid-solid multiphase reactions in geological materials to deduce the rate of crystal uplift
5:40 pm - 6:00 pm	M. Athenes Kinetics of phase separation in a binary alloy: influence of the atomic mobilities
6:00 pm - 6:20 pm	K. Rajan Self Assembly in epitaxial semiconductor alloys
6:20 pm - 6:40 pm	P. A. Khorzhavyi <i>Ab initio</i> study of vacancies in metals and compounds
6:40 pm - 7:00 pm	W. Pfeiler Point defect energies in L₁₂-ordered Ni₃Al
7:00 pm - 7:15 pm	Discussion
7:30 pm - 9:00 pm	Dinner
9:00 pm - 10:00 pm	Social Hour

Tuesday, August 10, 1999

7:00 am - 8:00 am Breakfast

Session IC: Thermodynamics of Alloys : phase stability and transformation

Chairperson: W. E. Glassley

8:00 am - 8:40 am S. Saxena
Application of synchrotron light, CCD-devices and lasers to the study of materials

8:40 am - 9:00 am K. Masuda-Jindo
Effects of continuous atomic displacement on the phase stability of metallic alloys

9:00 am - 9:20 am G. Grimvall
Dynamical lattice instabilities in alloy phase diagrams

9:20 am - 9:40 am S. Fries
Computational thermodynamics: modelling and applications

9:40 am - 10:00 am T. Mohri
Susceptibility near the transition temperature calculated from first-principles

10:00 am - 10:30 am **Coffee Break**

Chairperson: D. Papaconstantopoulos

10:30 am - 11:10 am W. Schweika
Diffuse scattering of Cu-Au alloys: displacements and Fermi-surface effects

11:10 am - 11:30 am V. Vinograd
Maximization of cluster entropy via an irreversible algorithm: application to the cluster variation method

11:30 am - 11:50 am C. Colinet
CVM calculations of the solid-state equilibria in the Fe-Co phase diagram

11:50 am - 12:10 pm S. Shallcross
Onsager cavity field in statistical mechanics of alloys

Tuesday, August 10, 1999 (continued)

12:30 pm - 2:00 pm	Lunch
2:00 pm - 5:15 pm	<i>Ad hoc</i> sessions and/or free time
5:15 pm	Coffee Service

Session II: Focused Session on Surfaces and Multilayers

Chairperson: J. S. Faulkner

5:30 pm - 5:50 pm	A. V. Ruban Random surface alloys: CPA versus super-cell approach
5:50 pm - 6:30 pm	S. Mahajan Two-dimensional phase separation and atomic ordering in mixed III-V layers
6:30 pm - 6:50 pm	Z. Chen The evaluation of the fracture strain of ITO films on polymeric substrates
6:50 pm - 7:30 pm	Discussion
7:45 pm - 9:15 pm	Dinner
9:15 pm - 10:15 pm	Social Hour

Wednesday, August 11, 1999

07:00 am - 09:00 am Breakfast

Session II: Focused Session on Surfaces and Multilayers

Chairperson: T. Mohri

8:00 am - 8:40 am J. Kudrnovsky
***Ab initio* theory of perpendicular transport in
magnetic multilayers**

8:40 am - 9:20 am J. Rustad
**Molecular dynamics simulation of iron oxide-water
interfaces with classical potentials**

9:20 am - 9:50 am Coffee Break

Session IC: Thermodynamics of Alloys : phase stability and transformation

Chairperson: K. Rajan

9:50 am - 10:30 am J. Wong
**In-situ chemical dynamics and phase
transformation under steep thermal gradients
using time-resolved and spatially resolved
diffraction**

10:30 am - 10:50 am B. Bokhonov
**Application of transmission electron microscopy
for in situ studies of the formation of intermetallic
compounds**

10:50 am - 11:10 am A. V. Ruban
**Crystal-structure effect in transition metals and
alloys**

11:10 am - 11:30 am M. Gubinsky
**One-stage Copper alloy recuperation from
bimetallic pipe waste**

12:00 noon - 7:30 pm Boxed Lunch and Optional Excursion

Wednesday, August 11, 1999 (continued)

19:00 - 20:30

Dinner

20:30 - 21:30

Social Hour

Thursday, August 12, 1999

7:00 am - 8:00 am Breakfast

Session III: Electronic Structure and Properties

Chairperson: W. H. Butler

8:00 am - 8:40 am J. S. Faulkner
Tests of the polymorphous coherent potential approximation

8:40 am - 9:20 am A. Lodder
Electromigration and electronic structure

9:20 am - 9:40 am T. C. Schulthess
Electronic structure and antiferromagnetic ordering in FCC FeMn

9:40 am - 10:00 am V. Milman
***Ab initio* study of Aluminosilicate garnets: structure, compressibility, and site disorder**

10:00 am - 10:30 am Coffee Break

Session III: Electronic Structure and Properties

Chairperson: S. G. Fries

10:30 am - 11:10 am D. Papaconstantopoulos
Tight-binding method for metals insulators and semiconductors

11:10 am - 11:30 pm B. Klein
A real-space, finite element approach to large scale electronic structure calculations

11:30 pm - 11:50 pm S. Znam
Bond-order potentials for transition metal based binary alloys:titanium-aluminum alloys

11:50 pm - 12:10 pm M. Menon
Tight-binding molecular-dynamics studies of relaxation around copper substitutional additive in Ni

12:10 pm - 12:30 pm P. James
***Ab initio* calculations of 3d alloys**

12:45 pm - 2:00 pm Lunch

Thursday, August 12, 1999 (continued)

2:00 pm - 4:45 pm *Ad hoc* sessions and/or free time

4:45 pm Coffee Service

Session IV: Mechanical Properties

Chairperson: P. E. A. Turchi

5:00 pm - 5:40 pm A. Lozovoi
Point defects in Al-rich NiAl alloys under pressure

5:40 pm - 6:00 pm H. Kokawa
Grain boundary structure dependence of carbide precipitation in sensitized austenitic stainless steel

6:00 pm - 6:20 pm T. Watanabe
Grain boundary engineering for the control of structure-dependent intergranular oxidation and fracture in nickel-40at% iron alloy

6:20 pm - 6:40 pm S. Hanada
Deformation and fracture of TiC/Mo(Nb) in-situ composites

6:40 pm - 7:00 pm A. Ohta
Doubled fatigued strength of box welds using low transformation temperature welding material

7:45 pm - 9:45 pm Conference Banquet

9:45 pm - 11:00 pm Social Hour

Friday, June 25, 1999

7:00 am - 9:00 am Breakfast

Session II: Focused Session on Surfaces and Multilayers

Chairperson: A. Gonis

8:00 am - 8:40 am W. H. Butler
Electronic transport in disordered magnetic multilayers

8:40 am - 9:20 am B. L. Györfy
Oscillatory magnetic coupling across alloy spacers in metallic multilayers and the corresponding Fermi surface

9:20 am - 10:00 am J. Tobin
Elementally specific magnetometry of alloys: surfaces and ultra thin films

10:00 am -10:15 am Gonis, Meike, Rajan, Turchi
Conference Close

12:00 noon Lunch (or boxed lunch by prior sign-up)

Poster: Surfaces and Multilayers

M. Yandouzi
Thin films NiAl evaporated onto Ag/NaCl study by CTEM and HRTEM

Second International Alloy Conference (IAC-2)
Oral Presentation

DYNAMICAL LATTICE INSTABILITIES IN ALLOY PHASE DIAGRAMS

Goran Grimvall, Theoretical Physics
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Ab initio electron structure calculations have been widely used to calculate the ground state energy of elements and compounds in various simple lattice structures, and thus account for the observed equilibrium structure. In the early 1990's it was noted that several of the metastable structures of the elements were in fact dynamically unstable under shear. For instance, W has the bcc structure, while fcc W has $c' < 0$. Similarly, Os has the fcc structure but a dynamically unstable bcc lattice with $c' < 0$. Here c' is Zener's elastic shear constant. With further progress in ab initio calculations, the phonon frequencies $\omega(\mathbf{q},s)$ could be accurately obtained in the entire Brillouin zone. Dynamical instabilities, i.e. $\omega^2 < 0$, were frequently found in many lattice structures of high symmetry. This paper discusses our present knowledge about dynamical lattice instabilities in elements, alloys and simple compounds. W-Re alloys are chosen as an illustrating example of the implications for the equilibrium composition-temperature phase diagram.

Second International Alloy Conference (IAC-2)
Oral Presentation

COMPUTATIONAL THERMODYNAMICS: MODELLING AND APPLICATIONS

Suzana G. Fries, ACCESS e.V., RWTH-Aachen
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W. Alan Oates, Science Research Institute, University of Salford, Salford M5 4WT, U.K

Thermodynamic databases constructed using the CALPHAD method consist in sets of empirically modelled Gibbs energy functions describing the phases existing in a given multicomponent system.

One advantage of these Gibbsian databases is to be able to calculate phase diagrams (and other thermodynamic properties) which reproduce experimental evidences found in commercial alloys with the precision required by technological applications.

The state of the art of First Principles calculated phase diagram, the theoretical alternative for treating phase stability, is still faraway of such a precision, leaving computational thermodynamics a successful and unique approach for these applications.

An overview will be given about the existing databases, models used, their link to materials, their use in simulations and the improvements that can be achieved if applications, pragmatic and theoretical approaches can unite.

Second International Alloy Conference (IAC-2)
Oral Presentation

**SUSCEPTIBILITY NEAR THE TRANSITION TEMPERATURE CALCULATED
FROM FIRST-PRINCIPLES**

Tetsuo Mohri, Division of Materials Science and Engineering, Hokkaido University
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There are several experimental evidences of slowing down behavior near the transition temperature for the first-order transition. In order to distinguish it from the conventional critical slowing down phenomenon, they call this as pseudo-critical slowing down phenomenon. The present work is undertaken to reveal the thermodynamic origin of this phenomenon. We employed Path Probability Method and obtained the temperature dependency of the relaxation time for L10-disorder transition. Then, further studied was attempted to calculate the generalized susceptibility near the transition temperature for Cu-Au system by combining Cluster Variation Method with electronic structure calculations. The results indicate that the susceptibility abruptly increases as approaching the transition temperature.

MAXIMIZATION OF CLUSTER ENTROPY VIA AN IRREVERSIBLE ALGORITHM: APPLICATION TO THE CLUSTER VARIATION METHOD. Victor L. Vinograd, Udo Becker, and Andrew Putnis, Institute of Mineralogy, University of Münster, Münster, Germany.

The main difficulty in the cluster variation method is the search for the global free energy minimum in a multi-dimensional space of cluster variables (correlation functions). In models which consider nearest-neighbor (*nn*) interactions only (those within pair, triangle or tetrahedron) the problem can be reduced to two separate tasks:

- 1) entropy maximization constrained by fixed *nn* correlation functions,
- 2) free energy minimization with respect to the *nn* correlation functions.

Our presentation shows that the first task can be further reduced to entropy maximization of a basic cluster, while the cluster entropy can be maximized via a set of irreversible operations on cluster probabilities. With the help of the irreversible algorithm the maximum cluster entropy can be found directly as a function of *nn* correlation functions, avoiding explicit introduction of correlation functions of higher-order.

The method allows easy evaluation of high-order CVM approximations for lattices of various topology. The accuracy of the method is discussed in relation to the two-dimensional (square lattice) Ising model.

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Second International Alloy Conference (IAC-2)
Oral Presentation

**CVM CALCULATION OF THE SOLID STATE EQUILIBRIA IN THE FE-CO PHASE
DIAGRAM**

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A. Antoni-Zdziobek, LTPCM / ENSEEG / INPG

Solid state phase equilibria in Fe-Co system are investigated using the CVM method in the irregular tetrahedron approximation in the bcc lattice and in the regular tetrahedron approximation in the fcc lattice. Calculations are performed in the quaternary Fe+Fe-Co+Co- by considering both chemical and magnetic interactions. The A2/B2 order/disorder transition and the alpha/gamma transition agree well with the experimental data in the literature. The composition dependence of the Curie temperatures for bcc and fcc alloys as predicted here are also presented.

Tuesday, August 10, 1999 (continued)

Session II: Focused Session on Surfaces and Multilayers

Chairperson: J. S. Faulkner

A. V. Ruban

Random surface alloys: CPA versus super-cell approach

S. Mahajan

Two-dimensional phase separation and atomic ordering in mixed III-V layers

Z. Chen

The evaluation of the fracture strain of ITO films on polymeric substrates

Second International Alloy Conference (IAC-2)
Oral Presentation

CRYSTAL-STRUCTURE EFFECT IN TRANSITION METALS AND ALLOYS

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H. L. Skriver, Danish Technical University

It is demonstrated that the crystal structure strongly influences thermodynamic properties such as solution, mixing and segregation energies in transition metal alloys. The origin of the strong structural effects is the local character of interatomic bonding which can be accounted for in the virtual-bond model. This model is discussed in application to the solution, mixing and segregation energies.

PHASE SEPARATION AND ATOMIC ORDERING IN MIXED III-V LAYERS

S. Mahajan

Department of Chemical, Bio and Materials Engineering and
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Tempe, AZ 85287-6006

ABSTRACT

It will be shown that atomic species in mixed III-V layers are not distributed at random on their respective sub-lattices. Two types of deviations from randomness are observed: phase separation and atomic ordering. Phase separation occurs on the surface while the layer is growing and is two-dimensional in nature. It cannot be suppressed using non-equilibrium growth techniques, is only observed in layers whose constituents differ in their tetrahedral radii, and its occurrence is governed by surface thermodynamics.

Atomic ordering coexists with phase separation in layers grown by vapor phase techniques. Depending on the prevailing surface reconstruction, double and triple period superlattices develop on {111} planes. It will be argued that the occurrence of surface reconstruction produces sub-surface stresses that bias the occupation of certain sites by atomic species differing in their tetrahedral radii, resulting in atomic ordering. Furthermore, the influence of phase separation and atomic ordering on electronic properties will be discussed.

Second International Alloy Conference (IAC-2)
Oral Presentation

THE EVALUATION OF THE FRACTURE STRAIN OF ITO FILMS ON POLYMERIC SUBSTRATES

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W. Wang, Institute of Materials Research and Engineering
B. Cotterell, Institute of Materials Research and Engineering

One of the mechanical issues concerning flexible organic light emitting device (OLED) is the flexibility, which is controlled by the fracture strength of the brittle films in the device. For example, the integrity of the anode material, the ITO film in the device directly controls the functioning of the device. Understanding the behaviour of these films under flexed condition will help maximize the flexibility of the device. Experiments have been devised to achieve this goal by bending the films of interests to gradually increased curvature over the point of film cracking, both under tension and compression. In this work concentration is given to ITO film. Fracture mechanisms under tension is found to be parallel channelling crack. Under compression the film fails by channelled buckling delamination prior to film cracking, which superficially looks very similar to the tensile cracking if observed under optical microscope or lower-resolution SEM. Based on the understanding of the thin film mechanics on the above phenomena, ways to improve the flexibility are proposed from device design point of view.

Wednesday, August 11, 1999

Session II: Focused Session on Surfaces and Multilayers

Chairperson: T. Mohri

J. Kudrnovsky

***Ab initio* theory of perpendicular transport in magnetic multilayers**

J. Rustad

Molecular dynamics simulation of iron oxide-water interfaces with classical potentials

Session IC: Thermodynamics of Alloys : phase stability and transformation

Chairperson: K. Rajan

J. Wong

In-situ chemical dynamics and phase transformation under steep thermal gradients using time-resolved and spatially resolved diffraction

B. Bokhonov

Application of transmission electron microscopy for in situ studies of the formation of intermetallic compounds

A. V. Ruban

Crystal-structure effect in transition metals and alloys

M. Gubinsky

One-stage Copper alloy recuperation from bimetallic pipe waste

ABSTRACT FOR IAC-2
August 8-13, 1999 - Davos, Switzerland

Submitted to main topic area: 1

Subtopic area: b. Conductivity/Transport

AB INITIO THEORY OF PERPENDICULAR TRANSPORT IN MAGNETIC MULTILAYERS, Josef Kudrnovský and Václav Drchal, Institute of Physics ASCR, Prague; Ilja Turek, Institute of Physics of Materials ASCR, Brno; Claudia Blaas and Peter Weinberger, Center for Materials Science, Vienna and Patrick Bruno, Max-Planck Institute for Microstructure Physics, Halle

The perpendicular magnetoconductance of a trilayer consisting from the sample sandwiched between two ideal leads is developed on *ab initio* level. The sample consists of two magnetic slabs separated by non-magnetic spacer metal. We employ the transmission matrix formulation of the conductance in the framework of the spin-polarized surface Green function technique which fully exploits layered nature of the problem. The electronic structure part of the problem is treated in the framework of the tight-binding linear muffin-tin orbital method generalized to layered systems. The formalism is extended to the case of lateral supercells with random arrangements of atoms in each sample layer which allows to treat both the ballistic and diffusive transport regimes on equal footing. An efficient method for evaluation of the supercell lead surface Green function is presented.

The formalism is applied to fcc-Co/Cu/Co(001) based trilayers with possible disorder of the substitutional type in the spacer, magnetic slabs, and at sample interfaces.

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Invited talk

Second International Alloy Conference (IAC-2)
Oral Presentation

**IN-SITU CHEMICAL DYNAMICS AND PHASE TRANSFORMATION UNDER STEEP
THERMAL GRADIENTS USING TIME-RESOLVED AND SPATIALLY RESOLVED
DIFFRACTION**

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Intense synchrotron x-radiation emitted from storage rings provides a number of novel experimental probes to study materials structure, synthesis and processing in both time and spatial regimes not readily possible with conventional x-ray sources. This paper describes a couple of such novel tools developed at LLNL for investigating the chemical dynamics and phase transformation during synthesis and materials processing in real time and in-situ with sub-millimeter spatial resolution. These are time resolved x-ray diffraction (TRXRD) and spatially resolved x-ray diffraction (SRXRD). Examples of high temperature solid combustion synthesis and phase mapping in the heat affected zone (HAZ) of fusion welds will be discussed in some detail. Future prospects for such in-situ material dynamics research with high brightness 3rd generation synchrotron sources will be outlined.

Second International Alloy Conference (IAC-2)
Oral Presentation

**APPLICATION OF TRANSMISSION ELECTRON MICROSCOPY FOR IN SITU
STUDIES OF THE FORMATION OF INTERMETALLIC COMPOUNDS.**

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In the present work, transmission electron microscopy was applied to the studies of structural and morphological characteristics during in situ interaction in metal systems. For this purpose, the pairs of interacting substances were chosen so that only one eutectic point was present in their phase diagrams Au-Si(Ge). Besides, the studies in the systems with unlimited solubility (Au-Ni, Cu-Au) and in the systems involving the formation of intermetallic compounds (Ni-Al, Au-Al, Ag-Al, Ni-Si, Ni-Ge) were also performed. Electron microscopic studies were carried out using the samples in which one of the interacting components was single crystal (or polycrystal) film or foil while the second component was present as a crystal particle of small size. The interaction between them was initiated with the help of a special heating unit or by the electron beam in the microscope with increased intensity. The application of this electron microscopic technique allowed us to obtain the data on the aggregate state of the reacting substances, the nature of transported particles and the ways of their transport; to reveal phase composition of the intermediate products and the sequence of stages through which the formation of the final product proceeds. Besides, the observations of the interaction allowed to make conclusions concerning the formation and the development of the defect structure at the interphase boundary between the interacting substances.

Second International Alloy Conference (IAC-2)
Poster Presentation

ONE-STAGE COPPER ALLOY RECUPERATION FROM BIMETALLIC PIPE WASTE

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The major disadvantages of the existing methods of copper alloys recuperation could be confined to the following factors: they result in a pronounced deterioration of a finished product quality, sufficient energy expenditure, multiple stages of production and irretrievable losses of such expensive alloying element as tin. Taking these shortcomings as a point of departure the authors assumed it vital to develop a highly efficient and simple technology of pyrometallurgical recycling of copper based alloys from bimetallic pipe waste.

The steel-copper and steel-bronze pipe production technology analysis shows that 1500 tons of copper-clad bimetallic pipe waste could be recuperated into 150 tons of recycled copper and alloys with the same amount of alloying components as that of virgin materials.

The technology is based on the melting temperature difference between steel and copper-based alloys. Different technological variants have been worked out for the technological temperature range between 1080-1130 C. Serial experiments allowed to define optimal values for the main technological parameters of the process: temperature and speed of heating, velocity of melt excision.

On the basis of experimental investigation the authors designed and tested a pilot unit for continuous non-ferrous metal recycling. The unit operation helped to specify technological regimes and to get representative batches of recycled bronze the content of which was identical to that of a virgin material.

Thursday, August 12, 1999

Session III: *Electronic Structure and Properties*

Chairperson: W. H. Butler

J. S. Faulkner

Tests of the polymorphous coherent potential approximation

A. Lodder

Electromigration and electronic structure

T. C. Schulthess

Electronic structure and antiferromagnetic ordering in FCC FeMn

V. Milman

***Ab initio* study of Aluminosilicate garnets: structure, compressibility, and site disorder**

Session III: *Electronic Structure and Properties*

Chairperson: S. G. Fries

D. Papaconstantopoulos

Tight-binding method for metals insulators and semiconductors

B. Klein

A real-space, finite element approach to large scale electronic structure calculations

S. Znam

Bond-order potentials for transition metal based binary alloys: titanium-aluminum alloys

M. Menon

Tight-binding molecular-dynamics studies of relaxation around copper substitutional additive in Ni

P. James

***Ab initio* calculations of 3d alloys**

Alloy Conference

Submitted to main topic area: 1. Electronic structure and properties

Subtopic area: b. Conductivity/transport

ELECTROMIGRATION AND ELECTRONIC STRUCTURE

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Regarding the two different contributions to the driving force, the direct force and the wind force, the rôle of the electronic structure has been quite different for the two. For the wind force increasingly sophisticated descriptions have been used, namely pseudopotential models, finite cluster models and, at the end, an ab initio Korringa-Kohn-Rostoker Green's function description. We will illustrate this by showing for which systems by now the wind force has been calculated, which include almost all FCC and BCC metals, while both self-electromigration and impurity migration have been treated. Some new results will be presented as well, which simulate electromigration along a grain boundary and over a surface. The direct force, on the other hand, has mainly been discussed in terms of the simple free electron, or jellium model. However, it will be shown that we have arrived at a point, at which more sophisticated descriptions of the electronic structure involved are becoming important. A recent analysis of new experimental results leads to the conclusion, that a migrating hydrogen atom effectively can have a direct valence smaller than unity, depending on the metal studied. By this it becomes challenging to perform calculations of the electronic structure of an interstitial, not only at its equilibrium position, but also at positions lying along the jump path. The barriers for doing so have been abolished recently, since a formulation has been found by which the free electron poles of the interstitial Green's function have become handable.

Second International Alloy Conference (IAC-2)
Oral Presentation

**ELECTRONIC STRUCTURE AND ANTIFERROMAGNETIC ORDERING IN FCC
FEMN**

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FCC FeMn is a chemically disordered but antiferromagnetically ordered alloy with face centered cubic structure. These seemingly contradicting facts can be understood in the light of non-collinear magnetic ordering and a first principles treatment of the electronic structure. We use the layer-KKR multiple scattering approach in conjunction with the single site CPA which we have generalized to allow for non-collinear alignment of the moments. We find that three magnetic states could be converged: The collinear 1Q state with alternating (100) planes that are compensated and the non-collinear 2Q and 3Q states, with four ferromagnetic sub-lattices that have their moments pointing along, respectively, the diagonals of the (100) face or along the diagonals of the cube. Both non-collinear states are stable with the 3Q state having the lowest energy. The collinear 1Q state is unstable. The partial densities of states of Fe and Mn are very similar in the non-collinear states with a pseudo gap forming at the Fermi level which in turn stabilizes antiferromagnetic ordering. Research sponsored by the Office of Basic Energy Sciences of the USDOE under contract DE-AC05-96OR22464 with Lockheed Martin Energy Research Corporation. SM and GJM are sponsored by NSF-DMR-94400399 and DOD nano structures DAAH-94-96-1-0316.

Second International Alloy Conference (IAC-2)
Oral Presentation

**AB INITIO STUDY OF ALUMINOSILICATE GARNETS: STRUCTURE,
COMPRESSIBILITY, AND SITE DISORDER**

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The structural and electronic properties of end-members of the aluminosilicate garnet family (pyrope, grossular, spessartine and almandine) have been investigated as a function of applied pressure. The study has been performed with the density-functional theory code CASTEP which uses pseudopotentials and plane-wave basis set.

The geometrical parameters of the unit cells containing 80 atoms have been fully optimized. The calculated static geometry, bulk modulus and its pressure derivative are in good agreement with the available experimental data. It is shown that the bending of the Si-O-Al angle between the octahedra and tetrahedra is the main compression mechanism for all garnets studied. The non-monotonic dependence of bulk modulus on unit cell volume is explained in terms of differences in compression mechanism for AlO_6 octahedra.

Further, the bonding and dynamics of Mg in pyrope is investigated. The potential at Mg site is strongly anisotropic, and also anharmonic in one direction. The calculations confirm that there is no static 'subsite' disorder of the Mg in pyrope.

The effect of a hydrogarnet substitution, $SiO_4(OH)_4$, on structure and properties of pyrope and grossular is investigated.

Second International Alloy Conference (IAC-2)
Oral Presentation

DR

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TIGHT-BINDING METHOD FOR METALS INSULATORS AND SEMICONDUCTORS D. A. Papaconstantopoulos, Center for Computational Materials Science, Naval Research Laboratory, Washington, DC, USA Tight-binding total energy methods bridge the gap between highly accurate, but slow and memory consuming, first-principles density functional calculations and fast, compact, but less accurate atomistic potential methods. Over the past few years we have developed a highly accurate tight-binding method. The environmentally sensitive tight-binding parameters are determined by fitting to the bands structures and total energies of a small number (10-50) first-principles calculations. The resulting Hamiltonian is used to interpolate between these first-principles calculations, allowing highly accurate determinations of structural energy orderings, elastic constants, phonon frequencies, and surface energies. We have also developed computer programs which can use these parameters to do tight-binding molecular dynamics and to determine the electronic structure of a system. In this talk we show typical results for metals,insulators and semiconductors. This work is supported by the U.S. Office of Naval Research and the Department of Defense Common HPC Software Support Initiative (CHSSI) program. Tight-binding total energy methods bridge the gap between highly accurate, but slow and memory consuming, first-principles density functional calculations and fast, compact, but less accurate atomistic potential methods. Over the past few years we have developed a highly accurate tight-binding method. The environmentally sensitive tight-binding parameters are determined by fitting to the bands structures and total energies of a small number (10-50) first-principles calculations. The resulting Hamiltonian is used to interpolate between these first-principles calculations, allowing highly accurate determinations of structural energy orderings, elastic constants, phonon frequencies, and surface energies. We have also developed computer programs which can use these parameters to do tight-binding molecular dynamics and to determine the electronic structure of a system. In this talk we show typical results for metals,insulators and semiconductors. This work is supported by the U.S. Office of Naval Research and the Department of Defense Common HPC Software Support Initiative (CHSSI) program.

Second International Alloy Conference (IAC-2)
Oral Presentation

**A REAL-SPACE, FINITE ELEMENT APPROACH TO LARGE-SCALE ELECTRONIC
STRUCTURE CALCULATIONS**

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We present an approach to solid-state electronic-structure calculations based on the finite-element method. In this method, the basis functions are strictly local, piecewise polynomials. Because the basis is composed of polynomials, the method is completely general and its convergence can be controlled systematically. Because the basis functions are strictly local in real space, the method allows for variable resolution in real space; produces sparse, structured matrices, enabling the effective use of iterative solution methods; and is well suited to parallel implementation. The method thus combines the significant advantages of both real-space-grid and basis-oriented approaches and so promises to be particularly well suited for large, accurate ab initio calculations. We develop the theory of our approach, discuss advantages and disadvantages, and report initial results, including electronic band structures and details of the convergence of the method. We also present results of studies of positrons in solids using this method, including the calculation of positron lifetimes and comparisons with experiment.

Second International Alloy Conference (IAC-2)
Oral Presentation

**BOND-ORDER POTENTIALS FOR TRANSITION METAL BASED BINARY ALLOYS:
TI-AL AND MO-SI ALLOYS**

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Bond-order potentials (BOPs) for atomistic modelling of lattice defects in materials with mixed metallic and covalent bonding are derived within a parametrized tight-binding framework. BOP is an order N, fully real space method that does not require use of periodic boundary conditions. The cohesive energy is composed of the bond energy that contains the angular dependence of the atomic interactions, an environment dependent central-force many-body term representing the overlap repulsion arising from the valence sp electrons, and a pair potential term representing short-range repulsions. A condition of charge neutrality at individual atoms is employed as an ersatz for self-consistency. For transition metal based alloys BOPs are constructed in which only the valence d-electrons are retained explicitly on the transition metal sites and the p-electrons on the non-transition metal sites. A common feature of these materials is negative Cauchy pressure that is adequately reproduced owing to inclusion of the environmentally dependent term. The tight-binding parameters, the two-center hopping integrals, entering the bond part have been generated by first-principles LMTO calculations that established their transferability. While for Ti-Al alloys these parameters scale simply with the separation of the corresponding atoms, it is shown that in the case of Mo-Si alloys their environmental dependence must be included. Specific potentials for TiAl with the L10 structure are presented and tested by the following studies that have been made in parallel with ab initio calculations: Comparison of competing structures with the same stoichiometry and investigation of complex transformation paths between different structures.

Second International Alloy Conference (IAC-2)
Oral Presentation

**TIGHT-BINDING MOLECULAR-DYNAMICS STUDIES OF RELAXATION AROUND
COPPER SUBSTITUTIONAL ADDITIVE IN NICKEL**

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The tight-binding molecular-dynamics (TBMD) simulation scheme for magnetic materials is generalized to include interactions of complex hetero-atomic systems. The data base for fitting the parameters is obtained from $\{it\ ab\ initio\}$ results for small clusters using the density functional method and the single, double and triple coupled clusters method. Further data base is obtained from experimental results for the bulk solid. The formalism thus developed is used to study electronic properties and lattice relaxation around a substitutional copper atom in a magnetic nickel host.

Thursday, August 12, 1999 (continued)

Session IV: Mechanical Properties

Chairperson: P. E. A. Turchi

A. Lozovoi

Point defects in Al-rich NiAl alloys under pressure

H. Kokawa

Grain boundary structure dependence of carbide precipitation in sensitized austenitic stainless steel

T. Watanabe

Grain boundary engineering for the control of structure-dependent intergranular oxidation and fracture in nickel-40at% iron alloy

S. Hanada

Deformation and fracture of TiC/Mo(Nb) in-situ composites

A. Ohta

Doubled fatigued strength of box welds using low transformation temperature welding material

Second International Alloy Conference (IAC-2)
Oral Presentation

POINT DEFECTS IN AL-RICH NiAl ALLOYS UNDER PRESSURE

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We investigate the effect of elevated pressures and finite temperatures on the point defect statistics in Al-rich NiAl alloys, where elimination of structural vacancies at high pressure is expected. In doing so we use density functional theory to compute point-defect energies as a function of pressure, which are in turn used as input to the Wagner-Schottky model. We find that at about 200 kbar a change in the constitutional defect takes place from V_{Ni} to Al_{Ni} . We extend the Wagner-Schottky model by introducing elastic interactions between defects, which leads to the prediction of a qualitatively new phenomenon in the system, namely the appearance of an isostructural phase transition terminated at a critical point. Similar behaviour is expected in some other 3/2 Hume-Rothery electron compounds.

Second International Alloy Conference (IAC-2)
Oral Presentation

**GRAIN BOUNDARY STRUCTURE DEPENDENCE OF CARBIDE PRECIPITATION
IN SENSITIZED AUSTENITIC STAINLESS STEEL**

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Grain boundary carbide precipitation and intergranular corrosion in sensitized austenite stainless steel were examined by transmission electron microscopy(TEM) to clarify the effect of grain boundary structure on precipitation and corrosion. A type 304 steel which had been solutionized at 1350 K was heat-treated at temperatures of 800-1300 K. Oxalic acid etch and Strauss tests showed that the frequency of grain boundaries with M₂₃C₆ carbide precipitation and corroded boundaries increased with holding time at sensitizing temperatures. The grain boundary carbide precipitation was observed during heat treatment at 1000 K by TEM. Grain boundaries were characterized on the basis of the Coincidence Site Lattice(CSL) theory using electron diffraction Kikuchi patterns. The observations revealed that the propensity to intergranular precipitation depends strongly on the grain boundary structure. Carbide precipitates tend to be detected at grain boundaries with higher sigma-values or larger deviation angles from low sigma CSL misorientations. The border lines between precipitation and no precipitation can be drawn by a parameter of deviation angle divided by the maximum deviation angle by Brandon's criterion. The parameter of border line decreased with the increase in the holding time at 1000 K. This means that the more ordered boundary needs the longer time for carbide precipitation and corrosion than less ordered or random boundaries.

Second International Alloy Conference (IAC-2)
Oral Presentation

GRAIN BOUNDARY ENGINEERING FOR THE CONTROL OF STRUCTURE-DEPENDENT INTERGRANULAR OXIDATION AND FRACTURE IN NICKEL-40AT% IRON ALLOY

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The most recent studies of structure-dependent intergranular oxidation and of the grain boundary engineering for the control of oxidation-assisted brittleness in polycrystalline materials are discussed. In order to control oxidation-assisted intergranular fracture which is often an important source of intergranular brittleness of high temperature materials, the effects of grain boundary type and the grain boundary character distribution (GBCD) and grain boundary connectivity on intergranular oxidation and related fracture have been studied in nickel-40at% iron alloy. It has been found that intergranular oxidation occurs preferentially at high energy random boundaries, while low-energy special boundaries like low sigma coincidence boundaries, particularly sigma 3, 11, 19, 27, 31, are highly immune to intergranular oxidation in coarse-grained specimens of the alloy. The effect of grain boundary type and structure on intergranular oxidation was observed to be more significant at a low-oxygen pressure (26ppm O₂) than atmospheric pressure (1 atm O₂). The effects of the grain boundary character distribution (GBCD) and the grain boundary connectivity have also been studied in rapidly solidified and subsequently annealed polycrystalline ribbons produced by rapid solidification from the melt of the alloy. The frequency of the low energy special boundaries which are resistant to intergranular oxidation and fracture, was increased from 30% to 60% by annealing after rapid solidification. Particular importance of this investigation is the finding that oxidation-assisted intergranular fracture and brittleness of the polycrystalline material can be controlled by engineering the GBCD and the grain boundary connectivity in connection with the grain size.

DEFORMATION AND FRACTURE OF TiC/MO(Nb) IN-SITU COMPOSITES

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To develop structural materials at very high temperatures over operating temperatures of conventional Ni base superalloys, refractory metal Mo(Nb)-reinforced TiC in-situ composites have been investigated in this study. The isothermal section at elevated temperature of the Ti-Mo-C system shows that TiC(Mo) can be equilibrated with Mo(Ti) in the wide composition field, and a similar tendency can be found in Ti-Nb-C system. Based on these isothermal sections, in-situ composites with various compositions were synthesized by mixing of Nb, Mo and TiC powders followed by arc-melting, and mechanical properties were investigated in relation to their microstructure. Microstructure of arc-melted Mo-40TiC is composed of primary TiC particles and eutectic lamellae consisting of TiC and Mo. Eutectic lamellar structure disappears by substituting Nb for Mo. High temperature compressive strength of the in-situ composites arc-melted can be increased by increasing Mo content to a stress level higher than monolithic TiC at temperatures between 1200 and 1500C. Solidification microstructure is coarsened by directional solidification after arc-melting, which increases creep strength; under a fixed applied stress, minimum creep rate of the directionally solidified composite at 1500C is almost equal to that of conventional Ni base superalloy single crystals at 1100C. Annealing after arc-melting leads to precipitation of fine bcc Mo(Nb) particles in primary TiC particles, thereby reducing the length of cracks introduced by indentation. Directional solidification increases the spacing of bcc Mo(Nb) phase, which raises the fracture toughness at ambient temperature.

Second International Alloy Conference (IAC-2)
Oral Presentation

**DOUBLED FATIGUE STRENGTH OF BOX WELDS BY USING LOW
TRANSFORMATION TEMPERATURE WELDING MATERIAL**

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The low transformation temperature welding material is developed to improve the fatigue strength by introducing compressive residual stress around weld. The developed welding material which contains 10% chromium and 10% nickel, begins to transform from austenite to martensite at about 180 degree centigrade and finishes it at room temperature. During the transformation, the weld metal expands. This expansion induces the compressive residual stress around the welded part of 20 mm thick JIS SM490B steel plate. The magnitude of welding residual stress is estimated to be about -100 MPa for developed joint, while that is about 500 MPa for the conventional one. The stress ratio effect due to the compressive residual stress makes the fatigue strength doubled. The fatigue limit for conventional box welds is 65 MPa, while that for developed one is about 130 MPa.

Keywords: Steel, Fatigue, Improvement, Residual stress, Transformation

Friday, June 25, 1999

Session II: Focused Session on Surfaces and Multilayers

Chairperson: A. Gonis

W. H. Butler

Electronic transport in disordered magnetic multilayers

B. L. Györfy

Oscillatory magnetic coupling across alloy spacers in metallic multilayers and the corresponding Fermi surface

J. Tobin

Elementally specific magnetometry of alloys: surfaces and ultra thin films

Poster: Surfaces and Multilayers

M. Yandouzi

Thin films NiAl evaporated onto Ag/NaCl study by CTEM and HRTEM

Second International Alloy Conference (IAC-2)
Oral Presentation

.. ELECTRONIC TRANSPORT IN DISORDERED MAGNETIC MULTILAYERS

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Electronic transport in magnetic multilayers has received considerable attention since the discovery of the giant magnetoresistance (GMR) effect. Recently, there have been observations of very large values of GMR[1] in sputtered single crystalline films. These films are of interest to alloy theorists because they apparently are of sufficient perfection that the major process which limits the electron lifetime at low temperature is impurity or alloy scattering. In order to investigate this regime we have calculated the electrical resistivity and giant magnetoresistance of cobalt-copper (100)

Second International Alloy Conference (IAC-2)
Oral Presentation

PROF

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A theoretical model, based on the screened KKR formalism, is developed for studying the exchange interaction of two semi-infinite layers separated by a non-magnetic metallic spacer layer which is either pure metal or binary alloy. First applications of the model for pure Cu, as well as Cu-Ni and Cr-V alloy spacers are also presented.

Second International Alloy Conference (IAC-2)
Oral Presentation

ELEMENTALLY SPECIFIC MAGNETOMETRY OF ALLOYS: SURFACES AND ULTRA THIN FILMS

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Nanoscale magnetic systems such as Giant Magneto-Resistive (GMR) and Spin-Valve Materials are miniature, complex, multilayered structures composed of a variety of alloys and elements. To sort out the atomic scale structure-property relationships in such devices and their simplified analogs, elemental specificity is a necessity. Obviously, magnetic sensitivity is also required. One way to obtain a combination of these characteristics is to perform magnetic dichroism in core level spectroscopy, e.g. x-ray absorption [1,2] or photoelectron spectroscopy [3]. Typically, the chirality that gives rise to ferromagnetic sensitivity is induced via the use of circularly polarized x-rays. However, it is also possible to set up a vectorial chirality in angle resolved experiments such as photoemission, using linearly polarized x-rays. [4-7] Because of the intrinsic limitations [8] of the Sum Rule [9,10] based analyses of absorption data, we have taken a dual track approach based upon a combined analysis using Circular Dichroism in Absorption [11] and Linear Dichroism in Photoemission. [12,13] Particular emphasis will be placed upon the discussion of 3d magnetic binary alloys composed of Ni, Fe and Co and their structure - property relationships. [12] [1]Phys. Rev. Lett. 58, 737 (1987); Phys. Rev. Lett. 62, 2620 (1989). [2]Phys. Rev. B. 42, 7262 (1990). [3]Phys. Rev. Lett. 65, 492 (1990). [4]Phys. Rev. Lett. 70, 3479 (1993); Solid State Commun. 86 647 (1993). [5]Phys. Rev. B 49, 15 682 (1994); Solid State Commun. 90, 557 (1994). [6]Phys. Rev. B51, 609 (1995). [7]J. Appl. Phys. 79, 5626 (1996); J. Vac. Sci. Tech. B14, 3171 (1996). [8]Phys. Rev. B 52, 6530 (1995); Phys. Rev. Lett. 68, 3642 (1992). [9]Phys. Rev. Lett. 68, 1943 (1992). [10]Phys. Rev. Lett. 70, 694 (1993). [11]J. Vac. Sci. Tech. A 15, 2287 (1997). [12]Phys. Rev. Lett. 79, 5166 (1997). [13]Phys. Rev. Lett. 81, 1306 (1998).

ENGINEERING FOUNDATION CONFERENCES

Alloy Conference

Davos, SWITZERLAND
August 08, 1999 to August 13, 1999

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Abstract for IAC-2

Submitted to main topic area: 2. Thermodynamic properties
Subtopic area: 2.b. Ordering and phase transformations

ORDERED STATES AND PHASE TRANSITIONS IN INTER-METALLICS AND THIN METALLIC FILMS, R. Banerjee, S. Amancherla, S.A. Dregia, S. Banerjee*, and H.L. Fraser, Department of Materials Science and Engineering, Ohio State University, 2041 College Road, Columbus, OH 43210, USA. *BARC, Trombay, India

Intermetallic compounds have been the subject of great interest in the past several years as candidate materials in structural applications. Since useful versions of these materials will be alloyed such that their compositions will not represent stoichiometry, it is important to develop means of describing their ordered state. For example, it is important to know and also predict the site occupancies of the various alloying elements. In addition to bulk forms, these materials will find application as thin films or in multilayered configurations. Since it has been demonstrated in several systems that materials can undergo phase transitions as a function of scale, it is important for these types of materials that the occurrence of these possible transitions be determined and predicted. This paper addresses both of these problems and presents simple thermodynamic models which may be used as predictive tools.

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