

**SYMPOSIUM P:**

**MATERIALS THEORY, SIMULATIONS, AND  
PARALLEL ALGORITHMS**

**November 27 - December 1, 1995**

**Chairs**

**Efthimios Kaxiras**  
Department of Physics and  
Division of Applied Sciences  
Harvard University  
Cambridge, MA 02138  
(617) 495-7977

**Priya Vashishta**  
Concurrent Computing Laboratory  
for Materials Simulations  
Nicholson Hall  
Louisiana State University  
Baton Rouge, LA 70803-4001  
(504) 388-1157 or (504) 388-1342

**John Joannopoulos**  
Department of Physics  
Massachusetts Institute of Technology  
77 Massachusetts Avenue  
Cambridge, MA 02139  
(617) 253-4806

**Rajiv K. Kalia**  
Department of Physics and  
Concurrent Computing Laboratory  
for Materials Simulations  
Nicholson Hall  
Louisiana State University  
Baton Rouge, LA 70803-4001  
(504) 388-1112

**Symposium Support**

Office of Naval Research  
National Science Foundation

Proceedings published as Volume 408  
of the Materials Research Society  
Symposium Proceedings Series.

P1623

**FULL-POTENTIAL LMTO CALCULATION OF Ni/Ni<sub>3</sub>Al INTERFACE ENERGIES, D.L. Price, University of Memphis, and B.R. Cooper, West Virginia University**

Coherent Ni/Ni<sub>3</sub>Al interfaces are common in the nickel based superalloys, which by design contain Ni<sub>3</sub>Al precipitates. These precipitates have a significant effect on the mechanical properties of the alloys, and the interface energies, in turn, affect the morphology of the precipitates. We have performed a series of calculations of the Ni/Ni<sub>3</sub>Al interface, using our full-potential LMTO electronic structure method coupled with a supercell geometry, to obtain the ideal interface energy. We report here on the results of continued calculations, particularly on the effects of relaxation, lattice constant, and impurities upon the interface energy, and we examine the relationship of these to the electronic structure. This research has been supported by the NSF/West Virginia EPSCOR Project.

P1624

**POTENTIALS FROM EXACT INVERSION OF AB INITIO ENERGY DATA, M.Z. Bazant and E. Kucurus, Dept. of Physics, Harvard University, Cambridge, Massachusetts**

Don et al. have shown that ab initio cohesive energy vs. volume curves can be inverted to obtain radial pair potentials that reproduce the data. Their proof relies on expressing the energy as a sum of linear operations on the radial pair potential. By generalizing an alternate proof involving recursions that do not rely on linearity, it is possible, given assumed angular dependencies, to obtain all radial factors in many-body cluster expansions that reproduce a set of cohesive energy curves. One data curve is needed for each radial function, but, if additional curves are used, the equations are overdetermined and inconsistent, because the assumed angular form is never perfect. The consistency of the radial functions obtained by inverting multiple data sets, however, provides a quantitative measure of how well the functional form of the angular factor (not the just parameters) models the bonding preferences of the material in various environments. Such capability can guide the development of potentials for covalently bonded materials. The application of our formulas to silicon energy data demonstrates how an analytic tool for evaluating proposed functional forms is a useful supplement to the usual simulated annealing fit of potential parameters.

(1) A.E. Carlsson, C.D. Gelatt, Jr., and H. Ehrenreich, *Phil. Mag.*, **A**, **41**, 241-250 (1980)

P1625

**MOLECULAR DYNAMICS SIMULATIONS FOR Xe ABSORBED IN ZEOLITES, Jussi Kantola, Juhani Vaara, Tapio T. Rantala and Jukka Laipin, Department of Physical Sciences, University of Oulu, P.O. Box 333, FIN-90571 Oulu, Finland**

Microporous materials are widely used in chemical industry as molecular sieves or catalysts. Therefore, in addition to fundamental interest in examining crystalline solids with exceptionally large unit cells, these materials offer also practical problems to solve. In relation with experiments, noble gas atoms are suitable for probing the structure of porous materials; related adsorbate dynamics and distribution.

We have constructed models and carried out molecular dynamics simulations for Xe atoms adsorbed in two different types of zeolites, NaA (4A) and AlPO-11. The former consists of large cages connected to a three dimensional network and the latter forms small one-dimensional elliptical channels for adsorbate motion. Here, the main emphasis is put on the investigation of Xe-Xe, interactions and the contributions from the (anisotropic) environment. Available potential functions were tested against *ab initio* potentials.

NMR spectroscopy is an excellent tool for observation of both the dynamics and interactions of <sup>29</sup>Xe atoms adsorbed in zeolites. Therefore, to evaluate some relevant NMR observables, available interatomic nuclear shielding functions of <sup>29</sup>Xe were used. Nature of some possible adsorption sites was also investigated.

P1626

**FIRST-PRINCIPLES CALCULATION OF THE PHONON DISPERSION AND CUBIC ANHARMONIC FORCE-CONSTANT TENSOR OF SILICON, Young K. Park, A. A. Maradudin, and R. F. Wallis, University of California, Irvine, CA 92717; and Andrew A. Quong, Sandia National Laboratories, Livermore, CA 94551**

The phonon-dispersion curves and Fourier-transformed cubic anharmonic force-constant tensor for silicon have been calculated using the results of density-functional perturbation theory in conjunction with a nonlocal *ab initio* pseudopotential and the "2n+1" theorem of the perturbation theory suggested by Gonze and Vigneron<sup>1</sup>. The response of the conduction electrons to the field of the ions is obtained self-consistently. The calculated third-order anharmonic force-constant of silicon at some high-symmetry points of the Brillouin zone are compared with results obtained by the frozen-phonon method<sup>1</sup>.

This work was supported by NSF grant DMR 9319404, by the San Diego Supercomputing Center, and by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences, <sup>1</sup>X. Gonze and J.-P. Vigneron, *Phys. Rev. B* **39**, 13120, (1989).

P1627

**DEFECT STRUCTURE OF β NiAl USING THE BFS METHOD FOR ALLOYS, Guillermo Bozzolo, Analex Corporation, 3001 Aerospace Parkway, Brook Park, OH; Carlos Amador, Facultad de Química, Universidad Nacional Autónoma de México, Ciudad Universitaria, 04510 Distrito Federal, México; John Ferrante and Ronald D. Noebe, National Aeronautics and Space Administration, Lewis Research Center, Cleveland, OH**

The BFS method for alloys is applied to the study of the β-phase of the Ni-Al system, which exists over a range of stoichiometry from 45-60 at.-% Ni. At the stoichiometric composition NiAl should exist in a perfectly ordered B2 structure. Ni-rich alloys are characterized by antisite point defects (with Ni atoms in the Al sites) with a decrease in lattice parameter. On the Al-rich side of stoichiometry there is a steep decrease in lattice parameter and density with increasing Al content. The presence of vacancies in Ni sites would explain such behavior. Recent X-ray diffraction experiments suggest a richer structure; the evidence, while strongly favoring the presence of vacancies in Ni sites, also suggests the possibility of some vacancies in Al sites in a 3:1 ratio. Moreover, local ordering of vacant sites may be preferred over a random distribution of individual point defects.

Our BFS semiempirical method using first principles rather than experimental input models the non-stoichiometric β-NiAl at zero temperature and quantitatively reproduces the lattice parameter and density dependence with composition. The simulation allows for a detailed vacancy concentration in agreement with experimental data.

**SIMULATIONS OF THE STRUCTURE AND PROPERTIES OF THE POLYETHYLENE CRYSTAL SURFACE, J.L. Wilhelm and G.C. Rutledge, Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139**

It has been well established that linear, flexible chain polymers crystallized from dilute solution form lamellar crystals. Such crystals exhibit two distinct surfaces, known as lateral and fold surfaces, with crystal growth occurring through the addition of chain segments to the lateral surface. While most attention has focused on the nature of the fold surface, the structure and properties of the lateral surfaces exert a strong influence on crystal growth behavior. Several different polymer crystallization theories indeed predict that the kinetics of crystal growth and the morphology of the solution grown crystal are highly dependent upon the structure and properties of the lateral surface, as manifested in the lateral surface free energy. However, few rigorous studies have been conducted to quantify the structure and properties of the lateral surface in crystalline polymers.