CHARACTERIZATION OF DEFECT SOLIDS

FINAL REPORT

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Period of Performance 1/92 to 12/94

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I. Introduction:

The purpose of this research has been to develop new semi-empirical techniques to describe ceramics, alloys and metal ceramic interfaces with applications in mind that support the materials aspects of the high speed civil transport program (HCST). HCST requires methods that aid in the design of alloys and ceramics for new high strength, high temperature applications. Current theoretical methods are not capable of carrying out this mission. Hence, new accurate and more efficient theoretical techniques are needed to facilitate the design of new materials and the examination of their properties. This program concentrated on modelling ceramics, but also dealt with alloy properties to a lesser degree.

The primary accomplishment of this research was the development of a new equation of state (EOS) that models the energy - bond length relationship and includes terms that represent charge transfer between cations and anions. This primary goal was accomplished with great success. The new EOS has been used by researchers at the Naval Research Laboratory to develop a new semi-empirical method for calculating properties of ceramics and metal ceramic interfaces based on the embedded atom method. The results of the DDF research describing the binding energy relation was the enabling theoretical basis. Also the workers at Cleveland State and NASA Lewis have detailed an approach based on equivalent crystal theory as part of the DDF which is currently under development. In addition, initial results for using the Harris functional method have been developed. Finally, the techniques developed by us have proved useful for the study of high pressure properties of solids and have been used extensively by researchers in this field.

A number of significant accomplishments have been achieved in this modestly funded program. These are listed below along with a list of resulting journal articles, presentations and book chapters. Copies of publications resulting from this research which detail the technical approaches and results are attached.
II. Major Accomplishments (1/92 -12/94):
Research supported by this grant has resulted in the publication of seven papers in refereed technical journals, a review article in a monograph on material science entitled "A.S.M.E. monograph on Flight Vehicle Materials, Structures and Dynamic Technology - Assessment and Future Directions", a paper presented at the European Conference on Surface Science, a paper to be presented at the March 1995 meeting of the American Physical Society and the award of a M.S. in Physics to a student at Cleveland State University.

III. Summary of Principal Results:
1. Development of a new semi-empirical method for obtaining binding curves of systems with charge transfer (i.e. cohesive energy vs. lattice spacing curves for partially ionic solids), with application to ceramics and potentially to alloys of transition metals. This method forms the basis of extensive calculations carried out by a group at the Naval Research Laboratory on ceramics and ceramic-metal interfaces.

2. Development of a new high pressure equation of state (EOS) for systems with charge transfer from the cohesive energy expression. This EOS fits the experimental isothermal compression and shock wave P-V data to very high pressures (i.e. P < 135 GPa).

3. Characterization of high pressure phases of solids. This led to a method for obtaining the cohesive energy of a high pressure phase from the experimental data for a lower pressure phase.

4. An extensive survey was carried out of the surface energy of fcc and bcc alloys including relaxation of atoms in the vicinity of the surface.

5. Empirical relationships were obtained between the lattice constant, cohesive energy and bulk modulus for halides, oxides, sulfides, selenides, tellurides and alkali chalcogenides with the NaCl, CsCl, CaF and NaO structures.
6. A new method was derived for characterizing the pressure dependence of the melting temperature of solids. Application was made to alkali and silver halides, metals and rare gas solids.

7. Derivation of a general thermodynamic model for the properties of pressurized solids with application to metallic nanocrystals.

8. A generalized Vegard relationship, obeyed by the isothermal bulk modulus, elastic constants and temperature derivative of the bulk modulus, was obtained for mixed alkali halide crystals.

9. Calculation of the temperature dependence of the elastic constants and of the thermal expansion of alkali halide crystals.

IV. The research supported by the Director's Discretionary Fund Grant (1/92 - 6/94) has resulted in the following publications and presentations:

A: Publications


2. Global Expression for Representing Cohesive Energy Curves II.
   (Cohesive energy curves for Halides, Oxides, and Sulfides).

   (EOS for Halides, Oxides, and Sulfides from cohesive energy parameters).

4. Computational Techniques in Material Science at the Atomic Level.

5. Pressure Dependence of Melting Temperature of Halides.
6. Multilayer Relaxation and Surface Structure of Ordered Alloys
R. Kobistek, G. Bozzolo, J. Ferrante and H. Schlosser,
(*) Research by R. Kobistek is in partial fulfillment of an M.S. in Physics
at Cleveland State University.


8. Thermodynamic Model for Pressurized Solids

B. Presentations
1. Surface Energies of BCC and FCC Metallic Alloys
Paper presented by G. Bozzolo at the European Conference on Surface Science
in Warwick, England (8/93)
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2. Statistical Model for Mechanical Failure
M. Kaufman, H. Schlosser and J. Ferrante.
Paper to be presented at the 1955 March Meeting of the American Physical
Society in San Jose, Ca.

C. Work to be Submitted for Publication
1. Volume Dependence of the Product of the Expansion Coefficient and the
Isothermal Bulk Modulus and of the Gruneisen Parameter for Pressurized Solids.

2. Generalized Vegard Law Scaling in Mixed Alkali Halide Crystals

H. Schlosser and J. Ferrante, to be submitted to Journal of Physics and
Chemistry of Solids.


V. Work in Progress:

1. Generalization of semi-empirical ECT method to partially ionic solids.
   a. Surface energy calculations in partially ionic solids (i.e. MgO).
   b. Defects in partially ionic solids.

2. First principles calculations of inputs to generalized ECT.
   a. Tight binding calculations (i.e. Harrison).
   b. Harris potentials.


4. Application of thermodynamic model to description of defects in metals and to study of fracture in solids.
VI. Publications and Presentations resulting from research supported by NASA Summer Faculty Fellowship.

A. Papers
1. Universal Energy Relations and Metal/Ceramic Interfaces.
   J.R. Smith, H. Schlosser, and J. Ferrante,

2. Rare Gas Liquids: Equation of State and Reduced Pressure Bulk-Modulus, and Sound Velocity Functions.


4. Pressure Dependence of the Melting Temperature of Rare-Gas Solids.

5. The Analysis of High Pressure Experimental Data.


B. Presentations
1. H. Schlosser, J. Ferrante and J. R. Smith,
   A Simple Global Representation of Binding Curves,

2. J. Ferrante, H. Schlosser and J. R. Smith,
   Global Representation of Potential Curves for Diatomics with Charge Transfer,
   American Vacuum Society, 7' th North Coast Symposium, May 31, 1990, Cleveland, OH.
3. H. Schlosser, J. Ferrante and J. R. Smith,
   A Global Expression for Representing Cohesive Energy Curves,
   American Physical Society Meeting, March 18-22 1991, Cincinnati, OH.

4. J. Ferrante,
   Applications of the Universal Energy Relationship,
   Case - Western Reserve University Physics Colloquium, September 10 1991,
   Cleveland, OH.

5. J. Ferrante and H. Schlosser,
   Presentation at Air Force Office of Scientific Research – University of
   Michigan Workshop on "Developing Potentials for Atomistic Simulations",
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   A.G. Evans, M.F. Ashby and J.P. Hirth, (Pergamon Press, Oxford and

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