$\mathcal{N}$ 95- 17654

CHARACTERIZATION OF DEFECT SOLIDS

FINAL REPORT

Professor Herbert Schlosser

Physics Department

Cleveland State University

Cleveland, Ohio 44115

Period of Performance 1/92 to 12/94

Final Report on the Director's Discretionary Fund Grant
CHARACTERIZATION OF DEFECT SOLIDS   (1/92 -12/94)
Professor Herbert Schlosser
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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

1. Cohesive Energy - Lattice Constant and Bulk Modulus - Lattice Constant Relationships: Alkali Halides, Ag Halides, Tl Halides.
   H. Schlosser, Journal of Physics and Chemistry of Solids 53, 855 (1992).

2. Global Expression for Representing Cohesive Energy Curves II.
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  Surface Science 307-309, 390 (1994).

  (*) Research by R. Kobistek is in partial fulfillment of an M.S. in Physics
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8. Thermodynamic Model for Pressurized Solids

  M. Kaufman and H. Schlosser, Journal of Physics: Condensed Matter (in press)

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 Paper presented by G. Bozzolo at the European Conference on Surface Science

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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

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5. Iterative Procedure for Obtaining the Cohesive Energy of a High Pressure
    Phase. H. Schlosser, to be submitted to Physica Status Solidi.

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).
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3. Generalization of thermodynamic model for pressurized solids to
    partially ionic solids. Application to calculation of properties of
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