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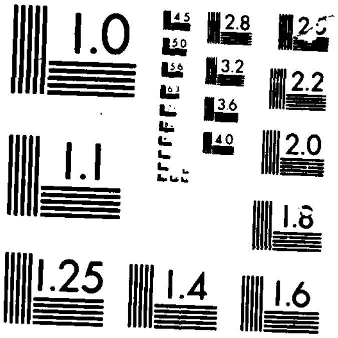

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The view, opinions, and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy, or decision, unless so designated by other documentation.

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Electron systems at arbitrary degeneracy; plasma states; shock Hugoniots; equation of state of aluminum; nuclear shock conditions; high pressure and electronic structure; high pressure structural probes

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This research has combined two major themes: the statistical mechanics of classical systems under conditions typical of shock or explosive environments, and the quantum statistical mechanics of inhomogeneous electron systems embedded in these classical ensembles. The project began with an application of the thermodynamics and structure of the liquid state, but applied in the context of a dynamic solid, [Jones and Ashcroft, J. Chem. Phys. 80, 3328 (1984)]. The method developed allowed us to reduce Hugoniot data to isotherms without the necessity of invoking any Grüneisen type of law. It was

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered) constructed explicitly for the case of insulating systems, but we were already able to see a possible modification for metals.

A system that seemed to remain very much an insulator under severe dynamic loading was SiO_2, whose band structure (in the fluorite phase) we calculated using the self-consistent augmented spherical wave method. The purpose of this calculation was to assess the result published by the Soviet group (Pavlovskii et al., 1978) which implied a dynamic collapse of SiO_2 under shock loading. One issue was whether such experiments should be repeated here (if for no other reason than to establish the actual shock capability of these experimenters). Our conclusion was that a density collapse of about a factor of four was necessary to account for the data, and this was unlikely on general theoretical grounds.

However, pressure as a general indicator of trends in electronic structure appears to be a tool of increasing value and versatility. For example, we were able to uniquely establish the sign of a pseudopotential coefficient for the simple element Al, a quantity that had been elusively resistant to determination. To do this we developed a method to analyze high pressure reflectivity data (Dandrea and Ashcroft, 1985) which also allowed us to infer the behavior of many-electron corrections to the band picture at elevated pressures. However, the major result of this work is that high pressure data has a lot to say about low pressure states of matter.

When high pressures are generated by shock methods, there is usually an accompanying increase in temperature, often very substantial. For nuclear driven shocks these temperatures can become so high that an electron system is driven far from degeneracy. When dealing with equation of state work, it is essential, therefore, to include finite temperature effects. Toward this end we have developed a theory of the high temperature electron fluid that actually is capable of taking us completely into the classical domain (Dandrea, Ashcroft, and Carlsson, 1986). We have presented closed form parametrizations for both thermodynamic functions and dielectric functions which give these quantitites over a complete range of density and temperature. This will be of considerable general use for those interested in high-temperature high-pressure equations of state for systems in which the electron gas forms a major contributor to the energy.

Dynamically Compressed Metals: Theory

FINAL REPORT

N. W. Ashcroft

April 15, 1986

U.S. ARMY RESEARCH OFFICE

DAAG 29-82-K-0170

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1. Foreward

The research supported by Grant DAAG 29-82-K-0170 during the period has dealt with the theory of condensed matter subjected to conditions of high pressure, high temperature, or both. These conditions are met during dynamic loading in chemical, mechanical, or nuclear shocks, and the corresponding conditions are appropriate to detonation pressures and high strain rate phenomena. In most of these the electron system, which we have studied in considerable detail, can still be viewed as in equilibrium. However the question of equilibrium for the atomic or ionic systems depends very much on circumstance. The research to be described below focuses mainly on the electron system since the required properties are common to most practical applications. However, we have taken this system into regimes that are far from degenerate, as will be described in the report below.

2(a). Problems Studied

This research has been directed towards problems in the general area of solids subjected to high pressures and high temperatures, conditions that are normally encountered in dynamic compression methods. These are as follows:

2(a)(i) Theory of the shocked solid: the statistical mechanics of solids viewed in the context of the liquid state.

2(a)(ii) Theory of electron bands in solids subjected to conditions of dynamic loading.

2(a)(iii) Pressure dependence of electron structure in simple metallic systems; inverting high pressure data to get fundamental interactions.

2(a)(iv) Theory of the high temperature and high density electron gas; charged interacting Fermions at arbitrary degeneracy.

2(b) Summary of Important Results

2(b)(i) It is well known that solids possess substantial cohesive energies in general. However the differences in energies between the various possible structures that a solid might assume are, by comparison, very much smaller. Taking this notion a step further, we can ask whether for structural purposes it may be sufficient to take the internal energy of a dynamic crystalline solid to be essentially that of a fluid phase at the same density. Since the fluid phase is homogeneous, this view has considerable analytical advantages.

We were able to show (1) that the view is valid and we successfully applied the ensuing formulation of the statistical mechanics of crystalline solids to the reduction of Hugoniots to isotherms. This approach, in inverse form, allows us to infer the properties of the short range interactions between atoms, the starting information coming from shock data.

2(b)(ii) Quartz is a well studied piezoelectric substance, both in the static and dynamic context. It is thought to remain in the insulating state under quite extreme shock conditions. However, though no substantial change in conductive properties have been announced, a rather dramatic collapse to a higher density phase has been reported by a Soviet Group (Pavlowskii et al.). If this were to be correct, the implications for possible structural collapse in other light element compounds would be profound. In order to assess the likelihood of core collapse in SiO_2, we examined the equation of state of this material at high density and when placed in a variety of different structures. The Soviet shock wave data seemed to indicate a collapse of about a factor of 4 in density. We found no indication of this at all in the theoretical results. These were obtained by the augmented spherical wave method, and while it might be argued that this technique is necessarily approximate, its application to the equation of state in other systems has proven to be quite satisfactory. Accordingly, the reported dynamic collapse in SiO_2 appears to be in doubt, although it can always be argued that non-equilibrium structures of great complexity are perhaps dominating the thermodynamic functions. This must be viewed, however, as unlikely.

2(b)(iii). Some features of electronic structure reveal themselves with great clarity. Thus in the polyvalent simple metals, the joint optical density of states is singular on account of a band structure property that owes its special form to zone symmetry. The singular structure is quite apparent in the frequency dependent reflectivity (as a sharp dip) and as the band structure is caused to change, so does the reflectivity. These changes can be brought about by application of pressure, so that turning the problem around, pressure dependence of the optical properties of a system can become a potent diagnostic and probe of electron structure. Our work has turned this general concept into an operational procedure, starting with Al as a trial system and using diamond anvil cell results which have so far produced compressions of about 22% in Al. We were also able to show that the method is capable of revealing effects beyond the independent electron (single-particle band-structure) model. One especially interesting future application will be towards dynamic systems under conditions that just precede melting. A measurement of the frequency dependent instantaneous absorptivity will give the interband absorption features, once again, but then will reflect the crystalline environment just prior to the solid-liquid instability. The connection between electron structure and density has been established by our grant research.

2(b)(iv) The dynamic-compression of metals is currently being achieved through the use of flying-plate (gas-gun) methods, through direct chemical shocks, and—especially for pressures in the multi-megabar region—nuclear shocks. In all of these techniques the delivery of substantial amounts of energy to the sample in a brief span of time results in rapid heating of the system. Accordingly, though high pressures are generated, they are often accompanied by extremely high temperatures, these reaching several electron volts (according to system). These conditions are obviously of considerable practical interest a range of materials problems. However, the combination of high temperature and high pressure is also quite characteristic of much of the material in the Universe and for this reason the fundamental aspects of this problem are of especial interest. Actually the properties of interacting electron systems in the range where temperatures approach or actually exceed the local Fermi energy has been an especially challenging one, but a challenge that we have evidently met. In a variety of forms this system underlies the behavior of the thermodynamic function and mechanical properties of all systems. We have therefore taken the theory of this system from the ground state, through the region of intermediate degeneracy, and then into the classical region where its properties merge with those of the classical one-component plasma. For those interested in the formulation of shock codes for dense, hot, matter, we have provided closed form parametric tabulations of both the thermodynamic functions of the dielectric function; equation of state and other thermodynamic quantities.

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2(c) List of Publications and Technical Reports

"The Electron Liquid at any Degeneracy," N. W. Ashcroft, R. G. Dandrea, A. E. Carlsson, March 1986 (submitted to Physical Review).

"Theory of the High Temperature Shocked Metallic State," N. W. Ashcroft, R. G. Dandrea, Proceedings of APS Conference on Shock Waves at Spokane, WA, July, 1985.

"Aluminum at $T \approx T_F$: Theory of the Dynamically Compressed Metallic State," N. W. Ashcroft, R. G. Dandrea, J. de Physique, Colloq. C8, 45, C8-13 (1984).

"High Pressure as a Probe of Electron Structure: Aluminum," N. W. Ashcroft, R. G. Dandrea, Phys. Rev. B 32, 6936 (1985).

"Properties of SiO_2 in a High-Pressure Fluorite Structure Phase," N. W. Ashcroft, A. R. Williams, A. E. Carlsson, Geophys. Res. Lett. 11, 617 (1984).

"Liquid State Thermodynamics and the Dynamic Compression of Solids," N. W. Ashcroft, R. S. Jones, J. Chem. Phys. 80, 7 (1984).

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