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The major theme of this research concerns the physics of systems that are subjected to conditions typical of shock or explosive environments. The focus is mainly but not exclusively on metallic systems; under shock loading they usually acquire a very substantial increase in temperature. In fact, for nuclear driven shocks the temperatures can become significant compared even with the Fermi temperature, and the systems are then taken quite far from degeneracy. Central to the theory of any metallic system is the physics of the underlying electron gas: what is required is a theory capable to giving its thermodynamic functions over a range spanning the extreme quantum to classical limits. Such a theory has been developed and under the present grant has been applied to nearly free electron metallic systems.

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22a. NAME OF RESPONSIBLE INDIVIDUAL N. W. Ashcroft

22b. TELEPHONE *(Include Area Code)* 607-255-8613

22c. OFFICE SYMBOL 529A Clark Hall

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Dynamically Compressed Metals: Theory

FINAL REPORT

N. W. Ashcroft

June 28, 1989

U.S. ARMY RESEARCH OFFICE

DAAL-03-86-K-0038

CORNELL UNIVERSITY

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1. Foreword

The research supported by Grant DAAL03-86-K-0038 during the funding period (1986-1989) has focussed on the theory of matter in the condensed state, but under conditions of extreme pressures, extreme temperatures, or both. These conditions are typical of samples subjected to dynamic loading, that is to shocks driven by mechanical, chemical, nuclear or laser means. They are most often encountered in detonation processes; all such dynamic techniques lead to non-equilibrium states of the atomic system. However because of their considerably lighter masses, the electron subsystem is often quite close to equilibrium. The research that will now be described deals with both equilibrium and non-equilibrium phenomena.

2(a). Problems Studied

2(a)(i) High temperature electron-systems. (This work was partially carried out under the previous grant, DAAG29-82-K-0170, and then developed and completed under the present grant.)

(2(a)(ii) Absolute scales for pressure at ultrahigh densities.

(2(a)(iii) Shock induced disorder and its influence on laser driven shock wave progression.

2(b) Summary of Important Results

2(b)(i) The major result of this research is the presentation of a unified theory that describes both the thermodynamic and dielectric properties of an interacting electron fluid throughout the full range of thermal degeneracy, that is, from the ground state (a degenerate Fermi plasma) to the classical domain where the system becomes a prototypical one-component plasma. In this work, we have obtained results that are quite accurate up to significantly large values of the coupling strength characteristic of the system. Furthermore, we have provided closed form parametrizations both of the thermodynamic functions, and of the dielectric response function of the electron gas over exceedingly large ranges of temperature and density. Since the electron gas is at the heart of the physics of the metallic state, these results, in parameterized forms, should be widely beneficial to a wide class of problem involving shocked metals. Finally, as ancilliary results, we have determined the effects of temperature on plasmon dispersion and damping in the electron gas. In the course of this work we discovered that quantum effects remain apparent to *surprisingly high temperatures*, indeed even for some plasma states that are traditionally regarded as classical!

2(b)(ii) In the last two years or so, there have been two reports in the literature of statically generated pressures in excess of 4 million atmospheres, a remarkable achievement if verifiable, and in terms of compression achieved one that is comparable to dynamic techniques. These conditions were produced in diamond cell devices, and the pressures reported were determined by the use of the observed shift of the ruby fluorescence line. However, the ruby scale is not an absolute scale; it ultimately has to be calibrated against a scale that is indeed truly absolute. For this reason, and because laboratory pressure ranges are approaching values of interest to planetary physicists and to research on high pressure materials synthesis, the issue of a fundamental and reproducible pressure scale in the range 0.1-1 Tpa (i.e. 1-10 megabar) becomes steadily more important.

In a collaborative effort with shockwave physicists at Los Alamos National Laboratory, this problem was tackled and solved. In fact, we were able to present absolute room temperature pressure scales in the range 1-10 mbar, as derived for the 3 metals Al, Cu, and Pb, so chosen because they conveniently overlap in pressure ranges covered. These 3 metals turn out to be extremely appropriate materials for pressure standards because much is known about their equations of state (partly from research carried out under this Grant and its predecessor) and because much is known theoretically about their electronic structures. In combination with recent shock data (including data obtained using nuclear impedance matching techniques) our theoretically determined thermodynamic functions for Al allowed this particular material to be used as a reference. Then the Hugonist curves for Pb and Cu could be determined from the impedance matching procedures. In the tabulated equations of state, the compressional reduction in volume actually exceeds, in the case of both Cu and Pb, an entire order of magnitude!

2(a)(iii) When a material is dynamically compressed, the constituent atoms, molecules, etc. are necessarily driven out of equilibrium. For mild or moderate shocks it is relatively common to assume that the states achieved by the system are not too far removed from equilibrium, so that in subsequent analysis local equilibrium states are often used. One interesting way of delivering moderate shocks in a reproducible way is to use pulsed power lasers (a pump-probe technique in which a shock front generated by one laser can be diagnostically probed by another). This technique has been used by some collaborators at the University of British Columbia in a detailed study of the behavior of fused quartz subjected to laser driven shocks. It has been discovered that the progression of the shock front is not in fact well described by an assumption of near-equilibrium conditions. To deal with this problem, we have introduced a model which far better accounts for the data. What is proposed is a new physical mechanism, namely irreversible shock induced disorder in the shock front. Because the local energy density is high, it is clear that bond re-orientation, production of local defects, and even bond disruption are examples of irreversible processes that can all have an impact on the entropy. Though initially adapted to quartz, some of the concepts introduced are of sufficient generality to be applicable to other polyatomic systems under shock loading conditions.

2(c) List of Publications and Technical Reports

"Non-Equilibrium Shock Behavior," A. Ng, B. K. Goodwal, J. Waterman, L. DaSilva, F. Cottet and N. W. Ashcroft, (to be published).

"Metals Physics at Ultrahigh Pressure: Aluminum, Copper, and Lead as Prototypes," W. J. Nellis, J. A. Moriarty, A. C. Mitchell, M. Ross, R. G. Dandrea and N. W. Ashcroft, N. C. Holmes and G. R. Gathers, Phys. Rev. Letts. 60, 1414 (1988).

"Electron Liquid at Any Degeneracy," R. G. Dandrea, N. W. Ashcroft and A. E. Carlsson, Phys. Rev. B 34, 2097 (1986).

2(d) Participating Scientific Personnel

1. N. W. Ashcroft Professor of Physics Cornell University Principal Investigator
2. R. G. Dandrea Graduate Research Assistant Cornell University
3. A. Denton Graduate Research Assistant (Summer Student)