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MASSACHUSETTS INSTITUTE OF TECHNOLOGY
CAMBRIDGE, MASSACHUSETTS 02139

TELEPHONE
(617) 864-1092

January 12, 1973

John M. Teen, Director, PR/HQ
ATTN: M. Hurvitz, Adm. Asst.
Contracts Branch

CONTRACT NO. AT(11-1)-3352 MASSACHUSETTS INSTITUTE OF TECHNOLOGY

We are transmitting copies of documents submitted in accordance with our requirements covering the subject contract.

(JK)

Philip Thompson, Contract Administrator
Contracts Division - Cambridge

CON-C:JK

Enclosures:

1. Ltr., Van Aken/Thompson, 12-13-72
2. Renewal Proposal (4) including:
Budget & 50 Word Scope of Work
3. Financial Statement (2)
4. SIE Form (3)
5. Progress Report No. C00-3352-4 (4)

cc: Brookhaven Patent Group - w/enc. 5
Division of Technical Information Extension, Oak Ridge, Tenn.,
(THRU BROOKHAVEN PATENT GROUP) - w/enc. 5 & AEC-427 form
Harold N Miller, Director, Contracts Division, CH - w/o enclosures

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Molecular Dynamics and Critical Phenomena in Liquids
and Solids

3. TYPE OF DOCUMENT (Check one):

- ☒ a. Scientific and technical report
☐ b. Conference paper not to be published in a journal:

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Date of conference _____

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Dr. S. H. CHEN Associate Prof. MIT

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Nuclear Engineering Dept.
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ANNUAL PROGRESS REPORT

to

Division of Research
United States Atomic Energy Commission

Thermal Neutron Scattering Studies of Molecular
Dynamics and Critical Phenomena in Fluids and Solids

AEC contract AT(11-1)3352
Period covered = December 1971-November 1972

Neutron Spectroscopy and Materials Research Group
Massachusetts Institute of Technology

Principal Investigator
Associate Investigator
DSR Staff
Research Assistants

Professor S.H. Chen
Professor S. Yip
Dr. L. Mistura
Y. Lefevre
T.A. Postol

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Contents

- I. Introduction
- II. Research Performed
 - IIa. Physics of Gaseous State
 - IIb. Physics of Liquid State
 - IIc. Additional Research Including Light Scattering
- III. References and List of Publications

MASTER

I. Introduction

The primary objective of this project continues to be the application of neutron inelastic-scattering spectroscopy to basic problems in materials science. The three-axis crystal spectrometer at the MIT research reactor has been in continuous operation for the last twelve months. From the stand point of the spectrometer the instrument is well suited for measuring quasielastic scattering at low energies. This is so because the double pyrolytic graphite monochromators are very efficient in extracting low energy neutrons which are free of second-order contamination. Also a detailed analysis of the resolution function has been carried out so that accurate corrections for instrumental resolution broadening are possible. From the standpoint of data analysis we are in a strong position with considerable in-house theoretical activities directed to study of time correlation functions in fluids. Thus there were both experimental and theoretical reasons for undertaking a program of line shape study of quasielastic peak. We have, in the eight months of spectrometer operation, performed rather detail measurements of hydrogen gas at 85°K and 300°K and pressures ranging up to 5000 psi; measurement on liquid gallium above and below the melting point.

Besides these experimental activities we have also initiated theoretical activities in both neutron and light scatterings. We organized an AEC Summer Institute on "Neutron Spectroscopy in Chemical Physics and Biophysics" and prepared a set of notes which we eventually hope to expand into a monograph. We shall in the following go into a little more detail of what we have done and give in each case the corresponding publications produced.

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II. Research Performed

IIa. Physics of gaseous state

Although neutron inelastic scattering has been used extensively to investigate liquid state dynamics, the related problem of the dynamical structure of gases has received very little attention. It is now generally recognized that a fundamental description of dynamic fluctuations in gases could be developed using kinetic theory. In particular, linear kinetic equations provide an essentially microscopic approach to the analysis of the scattering functions $S(Q, \omega)$ measured in neutron and light scattering experiments. Studies of this type are of fundamental interest because they represent a direct test of the foundations of current transport theories.

We have during the past year initiated a series of inelastic scattering experiments on pressurized hydrogen gas. The purpose was to study $S_s(Q, \omega)$ function for small values of Q to investigate the collisional narrowing in gases. The first attempt was carried out at 85°K with pressures ranging from 35, 70 to 140 atmosphere. The phenomena of collisional narrowing was observed for the first time and was successfully explained in terms of the kinetic theory. The paper was presented in the IAEA symposium on Neutron Inelastic Scattering at Grenoble in March (1972) ⁽¹⁾. Continuation of this measurement has since then produced data at 110, 120 and 130 atmosphere which besides showing improved agreement with the kinetic theory they further verify an important "scaling" property of the linearized Boltzmann equation. ⁽²⁾

Recently we have completed a set of measurement at 300°K and pressures up to 5000 psi. The result is being analysed, and will result in a M.S. thesis of P. Walsh.⁽³⁾

IIb. Physics of Liquid State

Our interest in the liquid state has so far centered in liquid metals and their mixtures. Gallium is a predominantly coherent scatterer so that we could measure $S(Q, \omega)$. First experiment we did was to measure the elastic diffraction pattern as a function of Q , namely $S(Q, \omega=0)$ which reflects the part of local atomic ordering which does not originate from thermal motions. We then formulate a theory which allows us to predict $S(Q, \omega=0)$ from the structure factor $S(Q)$. We found that the renormalized gas model gives a reasonable agreement with the experiment⁽⁴⁾. We next study $S(Q, \omega)$ above and below the melting point. We found no additional local ordering of atoms in the metastable supercooled state, compared to that of the normal liquid state. This implies that the instability is not caused by density fluctuations at or around the wave vector corresponding to the first diffraction peak as suggested by a recent theory. Analysis of the inelastic scattering spectra has shown that the concept of wave length dependent elastic moduli can play an equally important role in understanding the collective excitations that exist in either liquid insulators or liquid metals. The analysis was presented in the International Conference on Properties of Liquid Metals at Tokyo, September (1972)⁽⁵⁾. We have also analysed the data of Egelstaff and Cocking on liquid lead and sodium with the same theoretical model and satisfactory agreement was obtained⁽⁶⁾. Detail of both pressurized hydrogen gas and liquid gallium measurements are contained in a Ph.D thesis of Y. Lefevre⁽⁷⁾.

IIc. Additional Research including light scattering

Besides the neutron scattering activity S.H. Chen has been looking into possibilities of using the light scattering technique to do supplemental measurements of hydrodynamic and critical fluctuations in fluids. This appears very promising using a technique developed in our laboratory called "Light intensity correlation Spectroscopy." Three papers along this line have been written with support from this contract^{(8), (9), (10)}.

S. Yip has completed an article entitled "Spectral Measurement of Density Fluctuations in Fluid." This will appear as a chapter in a book edited by M. Velarde and M. Conlin Garcia⁽¹¹⁾.

III. References and a List of Publications

1. Y. Lefevre, S.H. Chen and S. Yip, "Translational Line Narrowing in Pressurized Hydrogen gas," paper presented at IAEA Symposium on Neutron Inelastic Scattering, Grenoble, France, March 1972, to appear as IAEA publication (1973).
2. S.H. Chen, Y. Lefevre and S. Yip, "Kinetic Theory of Collisional Line Narrowing in Pressurized Hydrogen Gas" (Manuscript to be sent to the Physical Review).
3. P. Walsh, "Neutron Scattering Study of Incoherent Scattering From Pressurized Hydrogen Gas at Room Temperature" M.S. thesis, M.I.T. (1973)
4. P. Ascarelli, S.H. Chen and R. Mical, "Coherent Neutron Elastic Scattering = Liquid Gallium" (Manuscript to be sent to the Physical Review).
5. S.H. Chen, Y. Lefevre and S. Yip, "Dynamics of Liquid Gallium in Supercooled State," paper presented at the Second International Conference on the Properties of Liquid Metals, Tokyo, September 1972, to be published in Phil. Mag. (1973).
6. C.H. Chung, S.Yip, and P.A. Egelstaff, "Dynamic Structure Factor Calculations and Neutron Inelastic Scattering". Paper presented at the Second International Conference on the Properties of Liquid Metals, Tokyo, September 1972, to appear in Phil. Mag. (1973).
7. Y.E.A. Lefevre, "Neutron Scattering Studies of Molecular Dynamics in Pressurized Gases and Liquid Metals." Ph.D thesis, MIT (1972).
8. P. Tartaglia, T.A. Pastol and S.H. Chen, "A Method For the Photocount Correlation Measurement." (Manuscript sent to J. Physics).
9. P. Tartaglia and S.H. Chen, "The Spacial Coherence Factor in Light Scattering From a System of Independent Particles." (Manuscript sent to Opt. Commun.).
10. P. Tartaglia and S.H. Chen, "Intensity Correlation of Light Scattered from Hydrodynamic Fluctuations" (Manuscript to be sent to J. Chem. Physics).
11. S. Yip, "Spectral Measurement of Density Fluctuations in Fluids." to appear as a Chapter in Thermodynamics and Statistical Physics (in Spanish) Vol. II, Edited by M. Velarde and M. Conlin-Garcia, Madrid (1973).