The Properties of Liquid Metals

THE PROPERTIES OF LIQUID METALS

Proceedings of the

SECOND INTERNATIONAL CONFERENCE

held at

Tokyo, Japan

3–8 September 1972

Editor

SAKAE TAKEUCHI

Director, The Research Institute for Iron, Steel and Other Metals, Tohoku University

Chairman of The Organizing Committee, The Science Council of Japan

TAYLOR & FRANCIS
LONDON

HALSTED PRESS
Division
JOHN WILEY & SONS
NEW YORK

1973

First published 1973 by Taylor & Francis Ltd., London and Halsted Press
(A division of John Wiley & Sons Inc.) New York, in association with the

Organizing Committee of LM2, The Science Council of Japan,
22–34 Roppongi 7-chome, Minato-ku, Tokyo, Japan.

Printed and bound in Great Britain by Taylor & Francis Ltd.,
10–14 Macklin Street, London WC2B 5NF.

Taylor & Francis ISBN 0 85066 065 3
Halsted Press ISBN 0 470-84414-0

Library of Congress Catalog Card number 73–1286

Distributed in Japan by Maruzen Co. Ltd.,
6 Tori-Nichome Nihonbashi, Tokyo 103.

The Conference was organized by The Science Council of Japan under the auspices of The Japan Institute of Metals, The Physical Society of Japan and The Iron and Steel Institute of Japan and under the sponsorship of The International Union of Pure and Applied Physics, and held at The Science Council of Japan, Tokyo, Japan, 3–8 September 1972.

THE PROPERTIES OF LIQUID METALS

Preface

The Second International Conference on the *Properties of Liquid Metals* was held in Tokyo, Japan, from 3 to 8 September 1972. It was organized by The Science Council of Japan under the auspices of The Japan Institute of Metals, The Physical Society of Japan and The Iron and Steel Institute of Japan, and was sponsored by The International Union of Pure and Applied Physics (IUPAP).

Because of the success of the first conference held at Brookhaven in 1966, it was hoped that a second conference would be given a warm reception. The main purpose of the most recent conference was to offer a chance to scientists, brought together from various fields of research, to have discussions centred on the physical properties of liquid metals and alloys. The main emphasis was on reports with regard to progress made in the intervening six years since the previous conference towards an understanding of liquid metals and alloys from the standpoint of much more refined atomic physics.

The conference was attended by one hundred and twenty-six Japanese and fifty-two foreign scientists from fifteen countries, and approximately one hundred and forty papers were submitted for presentation.

As can be seen from the contents of this volume, the fields represented ranged over the following five main subjects: Structure of liquid metals and alloys, Electronic states and electronic transport properties in liquid metals and alloys, Thermodynamic properties of liquid metals and alloys, Atomic transport properties in liquid metals and alloys, and Melting phenomena of metals. At the opening session Professor J. M. Ziman gave a lecture entitled "What do we not yet understand about liquid metals?" Sessions of each of the above subjects commenced with one or two reports in the nature of reviews summarizing progress in the relevant field since the first conference, followed by short contributions chosen mainly on the basis that they concerned recent research. All of the sessions were held in the lecture hall of The Science Council of Japan from 4 to 8 September 1972.

This volume contains eighty-four papers read at the conference including the opening lecture given by Professor J. M. Ziman and the talks of the nine specially invited speakers. In addition sixteen abstracts of papers from among those read by titles only are included. It is a great pleasure for me to include the report of Professor H. Ehrenreich as a special introduction to his field even though, to our regret, he did not, at the last moment, receive our invitation. His work concerns electronic states in alloys. The papers have been edited by the Organizing Committee prior to publication.

During the conference an informal meeting was called by the chairman of the Organizing Committee and attended by nine distinguished participants from abroad and members of the Organizing Committee. Its decision, announced on the last day of the Conference, was that a third conference on liquid metals be held in England, the tentative date to be sometime in 1976.

Last but not least I should like to take this opportunity, on behalf of the Organizing Committee, to acknowledge gratefully the financial support to the conference from numerous industrial and commercial organizations in Japan received through the efforts of the Finance Committee of The Japan Institute of Metals. Without such warm support the conference would certainly not have been so successful.

It is a pleasant duty for me as the chairman of the Organizing Committee to express my sincere thanks to the authors of the papers included in this volume, and also to the managing staff of the secretariat of The Japan Institute of Metals who so kindly cooperated with us in our attempt to make the conference a success.

SAKAE TAKEUCHI

1 December 1972 *Chairman of the Organizing Committee*

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List of participants

CANADA

BALLENTINE, Dr. L. E., Department of Physics, Simon Fraser University, Burnaby, B.C.
BHATIA, Prof. A. B., Department of Physics, University of Alberta, Edmonton, Alberta.
CROZIER, Dr. E. D., Department of Physics, Simon Fraser University, Burnaby, B.C.
EGELSTAFF, Prof. P. A., Department of Physics, University of Guelph, Guelph, Ontario.
MCALISTER, Dr. S. P., Department of Physics, Simon Fraser University, Burnaby, B.C.
TOUGAS, Prof. R., Ecole Polytechnique, 2500 Marie-Guyard Avenue, Montreal 250, P.Q.

FRANCE

RIALLAND, Mr. J. F., Laboratoire de Génie Electrique L.C.I.E., 33 Avenue du Général-Leclerc, 92 Fontenay-aux-Roses.
ROBERT, Prof. J., Laboratoire de Génie Electrique L.C.I.E., 33 Avenue du Général-Leclerc, 92 Fontenay-aux-Roses.
SCHIFF, Dr. D., Laboratoire de Physique Théorique et Hautes Energies, Bâtiment 211, Université de Paris, Centre d'Orsay, 91 Orsay.

GERMANY

BARTSCH, Prof. J., Technische University of Berlin, Institut für Metallkunde, 1000 Berlin 12.
GLÄSER, Dr. W. A., Institut für Angewandte Kernphysik, Kernforschungszentrum Karlsruhe, 75 Karlsruhe.
HENSEL, Prof. F., Institute of Physical Chemistry, Karlsruhe, University of Karlsruhe.
HOSEMANN, Prof. R., Fritz-Haber-Institut, 1-Berlin 33, Faradayweg 4–6.
PREDEL, Prof. B., Institut für Metallforschung, 44 Münster, Steinfurter Straße 107.
RUPPERSBERG, Prof. H., Institut Metallphysik & Metallkunde, Universität, D66, Saarbruecken.
STEEB, Dr. S., Max-Planck-Institut für Metallforschung, 7000 Stuttgart, Seestrasse 92.

HONG KONG

CHAN, Dr. J. P., Faculty of Natural Sciences and Engineering, Hong Kong Baptist College, 224 Waterloo Road, Kowloon.

INDIA

KUMAR, Dr. R., National Metallurgical Laboratory, Jamshedpur-7.

ISRAEL

GREENFIELD, Prof. A. J., Department of Physics, Bar-Ilan University, Ramat-Gan.
WISER, Prof. N., Department of Physics, Bar-Ilan University, Ramat-Gan.

ITALY

BORTOLANI, Prof. V., Instituto di Fisica dell'Università, Via Università, 4–41100, Modena.

JAPAN

ADACHI, Prof. Akira, Department of Metallurgy, Faculty of Engineering, Osaka University, Yamadakami, Suita, Osaka.
ADACHI, Prof. Kengo, Faculty of Engineering, Nagoya University, Chikusa-ku, Nagoya.
ASANO, Dr. Setsuro, The Institute for Solid State Physics, The University of Tokyo, Roppongi, Minato-ku, Tokyo.
ATSUMO, Mr. Eifu, 817 Moto Yoshida, Mito.
AZUMA, Dr. Masayoshi, Department of Physics, Faculty of Science, Niigata University, Ikarashi, Niigata.

BAJPAI, Dr. Ram Prakash, Research Institute for Catalysis, Hokkaido University, Sapporo.
CHIHARA, Mr. Junzo, Japan Atomic Energy Research Institute, Tokai-mura, Ibaraki.
DOYAMA, Prof. Masao, 3-37-2 Wakamiya, Nakano-ku, Tokyo.
EBISAWA, Dr. Hiromichi, Department of Applied Science, Faculty of Engineering, Tohoku University, Aoba, Sendai.
EJIMA, Prof. Tatsuhiko, Department of Metallurgy, Faculty of Engineering, Tohoku University, Aoba, Sendai.
EMI, Dr. Toshihiko, Research Laboratories, Kawasaki Steel Corporation, No. 1, Kawasaki-cho, Chiba.
ENDO, Prof. Hirohisa, Department of Physics, Faculty of Science, Kyoto University, Sakyo-ku, Kyoto.
FUKASE, Mr. Shoji, 4-10-5 Morisaki, Yokosuka.
FUKUDA, Dr. Kosaku, 3-27 Hishinumakaigan, Chigasaki, Kanagawa.
FUKUI, Mr. Yoshihiko, Department of Applied Science, Faculty of Engineering, Tohoku University, Aoba, Sendai.
FUKUSHIMA, Mr. Junichi, Department of Physics, University of Kyoto, Kitashirakawa, Oiwake-cho, Sakyo-ku, Kyoto.
FURUKAWA, Mr. Hiroshi, Department of Physics, Faculty of Science, Kyushu University, Fukuoka.
FURUKAWA, Dr. Kazuo, Tokai Laboratory, Japan Atomic Energy Research, Tokai-mura, Ibaraki.
FUWA, Prof. Tasuku, Department of Metallurgy, Faculty of Engineering, Tohoku University, Aoba, Sendai.
HAMAGUCHI, Dr. Yoshikazu, Physics Division, Japan Atomic Energy Research Institute, Tokai-mura, Ibaraki.
HARA, Mr. Hiroaki, Department of Applied Science, Faculty of Engineering, Tohoku University, Aoba, Sendai.
HASEGAWA, Dr. Masayuki, Department of Physics, Faculty of Science, Tohoku University, Katahira, Sendai.
HIROIKE, Prof. Kazuo, Department of Applied Science, Faculty of Engineering, Tohoku University, Aoba, Sendai.
HIRONE, President, Tokutaro, Yamagata University, Yamagata.
HIROTA, Prof. Toru, 26-2, 3-chome, Yurigaoka, Tama-ku, Kawasaki, Kanagawa.
HIWATARI, Dr. Yasuaki, Research Institute for Fundamental Physics, Kyoto University, Kyoto.
HOSHINO, Dr. Hideji, Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo.
IIDA, Mr. Keiichi, Faculty of Science, Niigata University, Ikarashi, Niigata.
IKEDA, Mr. Susumu, The Research Institute for Iron, Steel and Other Metals, Tohoku University, Katahira, Sendai.
INOUE, Mr. Shin-ichi, The Institute for Solid State Physics, The University of Tokyo, Roppongi, Minato-ku, Tokyo.
ISHIDA, Mr. Yoshiaki, Department of Applied Physics, Faculty of Science, Tokyo Institute of Technology, Meguro-ku, Tokyo.
ITAGAKI, Mr. Kimio, Research Institute of Mineral Dressing and Metallurgy, Tohoku University, Katahira, Sendai.
ITAMI, Dr. Toshio, Technical Research Laboratory, Kawasaki Steel Corporation, Chiba.
ITOH, Mr. Fumitake, The Research Institute for Iron, Steel and Other Metals, Tohoku University, Katahira, Sendai.
ITO, Mr. Kikuo, 1 Tanaka-Shimoyanagi-cho, Sakyo-ku, Kyoto.
IWAMOTO, Prof. Nobuya, Department of Metallurgy, Faculty of Engineering, Osaka University, Osaka.
KACHHAVA, Dr. Chauth, Research Institute for Catalysis, Hokkaido University, Sapporo.
KAI, Dr. Kenzo, The Research Institute for Iron, Steel and Other Metals, Toboku University, Katahira, Sendai.
KAMAKURA, Mr. Shiro, Department of Physics, College of General Education, Kyushu University, Fukuoka.
KAMIMURA, Prof. Hiroshi, Department of Physics, Faculty of Science, University of Tokyo, Bunkyo-ku, Tokyo.
KAMIYAMA, Mr. Tomoaki, The Research Institute for Iron, Steel and Other Metals, Tohoku University, Katahira, Sendai.
KANEYOSHI, Dr. T., Department of Physics, Nagoya University, Nagoya.
KASAMA, Mr. Akio, Department of Metallurgy, Faculty of Engineering, Osaka University, Yamadakami, Osaka.
KATAYAMA, Mr. Shin-ichi, Department of Physics, Niigata University, Ikarashi, Niigata.

KATO, Mr. Yoshiji, 38–6 Oiwake-cho, Kitashirakawa, Sakyo-ku, Kyoto.
KATSUTA, Dr. Hiroji, Japan Atomic Energy Research Institute, Tokaimura, Ibaraki.
KAWAI, Prof. Yasuji, Faculty of Engineering, Kyushu University, Hakozaki, Fukuoka.
KIKUCHI, Dr. Yoshikazu, Fibers & Textiles Research Laboratories, Toray Industries Inc., 3-chome, Sonoyama, Otsu.
KITA, Mr. Yoshifumi, Department of Metallurgy, Faculty of Engineering, Osaka University, Osaka.
KITAJIMA, Mr. Masahiro, Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo.
KOBAYASHI, Dr. Teiji, Department of Physics, Faculty of Science, Tohoku University, Katahira, Sendai.
KOJIMA, Mr. Kunihiro, Department of Pure and Applied Science, College of General Education, University of Tokyo, Komaba, Meguro-ku, Tokyo.
KURAMOTO, Mr. Yoshiki, Department of Physics, Faculty of Science, Kyushu University, Fukuoka.
MAEKAWA, Dr. Takashi, Faculty of Science, Hokkaido University, Sapporo.
MATSUDA, Prof. Hirotsugu, Research Institute for Fundamental Physics, Kyoto University, Sakyo-ku, Kyoto.
MATSUURA, Mr. Makoto, The Research Institute for Iron, Steel and Other Metals, Tohoku University, Katahira, Sendai.
MINOMURA, Prof. Shigeru, Institute for Solid State Physics, University of Tokyo, Roppongi, Minato-ku, Tokyo.
MISAWA, Mr. Masakatsu, The Research Institute for Iron, Steel and Other Metals, Tohoku University, Katahira, Sendai.
MISAWA, Prof. Setsuo, Department of Physics, College of Science and Engineeering, Nihon University, Kanda-Surugadai, Tokyo.
MORITA, Prof. Akira, Department of Physics, Faculty of Science, Tohoku University, Katahira, Sendai.
MORITA, Prof. Tohru, Department of Applied Science, Faculty of Engineering, Tohoku University, Aoba, Sendai.
MORITA, Prof. Zen-ichiro, Department of Metallurgy, Faculty of Engineering, Osaka University, Yamadakami, Osaka.
MURAKAMI, Mr. Katsuhiko, The Research Institute for Iron, Steel and Other Metals, Tohoku University, Katahira, Sendai.
MURASE, Dr. Chiaki, Department of Physics, College of General Education, University of Tokyo, Meguro-ku, Tokyo.
MURATA, Mr. Yoshiharu, International Department, Nihon Radiator Company, 5–24–15, Minami-dai, Nakano-ku, Tokyo.
NAKAGAWA, Prof. Yasuaki, The Research Institute for Iron, Steel and Other Metals, Tohoku University, Katahira, Sendai.
NAKAJIMA, Prof. Sadao, The Institute for Solid State Physics, University of Tokyo, Roppongi, Minato-ku, Tokyo.
NAKAMURA, Mr. Mitsunobu, Department of Electronic Engineering, Tamagawa University, Machida, Tokyo.
NAKAMURA, Prof. Yoshio, Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo.
NARA, Prof. Hisashi, Department of Physics, College of Arts and Science, Tohoku University, Kawauchi, Sendai.
NOGUCHI, Prof. Seiichiro, Faculty of Engineering, Nagoya University, Senju-ku, Nagoya.
OBATA, Dr. Yukio, Tokai Laboratory, Japan Atomic Energy Research Institute, Tokai-mura, Ibaraki.
OGAWA, Dr. Tohru, Department of Physics, Faculty of Science, Kyoto University, Kyoto.
OGITA, Dr. Naofumi, Institute of Physical and Chemical Research, Wako, Saitama.
OGURA, Mr. Hisakazu, Department of Physics, Faculty of Science, Kyoto University, Kyoto.
OKAJIMA, Prof. Kazuhisa, Department of Metallurgy, Faculty of Engineering, Nagoya University, Nagoya.
OKAZAKI, Mr. Hideo, College of General Education, Niigata University, Ikarashi, Niigata.
ONO, Prof. Syu, Institute of Physics, College of General Education, University of Tokyo, Komaba, Meguro-ku, Tokyo.
ONO, Prof. Yoichi, Faculty of Engineering, Kyushu University, Fukuoka.
OSHIMA, Mr. Ryuzo, Department of Physics, Faculty of Science, University of Kyoto, Kyoto.
OTSUKA, Mr. Shinya, Department of Metallurgy, Faculty of Engineering, Osaka University, Osaka.
OYA, Mr. Masato, Department of Applied Physics, Faculty of Engineering, Osaka University, Yamadakami, Suita, Osaka.

SAIKAWA, Dr. Kazuhiko, Department of Physics, Faculty of Science, Shinshu University, Matsumoto.
SAITO, Mr. Yasuo, Department of Chemical Engineering, Faculty of Engineering, Tohoku University, Aoba, Sendai.
SAKAMOTO, Mr. Masanobu, Physics Division, Japan Atomic Energy Research Institute, Tokai-mura, Ibaraki.
SASAKI, Mr. Ken, Japan Atomic Energy Research Institute, Tokai Research Establishment, Tokai-mura, Ibaraki.
SATOH, Prof. Takeshi, 16–16, 5-chome, Koyama, Shinagawa, Tokyo.
SENOO, Mr. Masagumi, Department of Mechanical Engineering, Nagoya University, Chikusa-ku, Nagoya.
SETOGAWA, Mr. Isao, B–4–1 Hashirimizu, 2-chome, Yokosuka.
SHIMADA, Mr. Katsumi, Department of Applied Physics, Osaka City University, Sumiyoshi-ku, Osaka.
SHIMOJI, Prof. Mitsuo, Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo.
SHIMOMURA, Mr. Osamu, Institute for Solid State Physics, Roppongi, Minato-ku, Tokyo.
SUNOSAKI, Mr. Masaru, Department of Metallurgy and Materials Science, Faculty of Engineering, The University of Tokyo, Bunkyo-ku, Tokyo.
SUZUKI, Prof. Hideji, Department of Physics, The University of Tokyo, Hongo, Bunkyo-ku, Tokyo.
SUZUKI, Mr. Hiroshi, Miyagi University of Education, Aramaki Aoba, Sendai.
SUZUKI, Prof. Kenji, The Research Institute for Iron, Steel and Other Metals, Tohoku University, Katahira, Sendai.
SUZUKI, Prof. Masuo, Institute for Solid State Physics, University of Tokyo, Roppongi, Minato-ku, Tokyo.
TAKEUCHI, Prof. Sakae, The Research Institute for Iron, Steel and Other Metals, Tohoku University, Katahira, Sendai.
TAKEUCHI, Mr. Takashi, Toyoda Physical and Chemical Research Institute, 2–13 Hisakata, Showa-ku, Nagoya.
TAKEYAMA, Dr. Kyozo, Department of Physics, Faculty of Science and Engineering, Chuo University, Bunkyo-ku, Tokyo.
TAMAKI, Prof. Shigeru, Department of Physics, Faculty of Science, Niigata University, Ikarashi, Niigata.
TAMURA, Mr. Kozaburo, Department of Physics, Faculty of Science, Kyoto University, Kyoto.
TANAKA, Prof. Minoru, Department of Applied Science, Faculty of Engineering, Tohoku University, Aoba, Sendai.
TANAKA, Miss Setsuko, Department of Physics, Faculty of Science, Aoyama University, Setagaya-ku, Tokyo.
TANEMURA, Mr. Masaharu, Department of Physics, Faculty of Science, University of Kyoto, Sakyo-ku, Kyoto.
TOKITA, Mr. Masahiko, Department of Applied Physics, Faculty of Engineering, Nagoya University, Nagoya.
TOKUDA, Prof. Taneki, 500 Kuji, Kawasaki.
TSUJI, Mr. Kazuhiko, Department of Physics, Faculty of Science, Kyoto University, Kyoto.
TSUCHIYA, Mr. Yoshimi, Department of Applied Physics, Nagoya University, Chikusa-ku, Nagoya.
UEDA, Prof. Akira, Department of Applied Mathematics and Physics, Kyoto University, Kyoto.
WASEDA, Mr. Yoshio, Research Institute of Mineral Dressing and Metallurgy, Tohoku University, Katahira, Sendai.
WATABE, Prof. Mitsuo, Department of Physics, Faculty of Science, Tohoku University, Katahira, Sendai.
YADA, Mr. Masaaki, 1037–8 Mukogaoka, Tokatsu-ku, Kawasaki.
YAMAMURA, Mr. Tsutomu, Department of Metallurgy, Faculty of Engineering, Tohoku University, Aoba, Sendai.
YAMASHITA, Prof. Jiro, Institute for Solid State Physics, University of Tokyo, Roppongi, Minato-ku, Tokyo.
YASUHARA, Dr. Hiroshi, College of Arts and Science, Tohoku University, Kawauchi, Sendai.
YAZAWA, Prof. Akira, Research Institute of Mineral Dressing and Metallurgy, Tohoku University, Katahira, Sendai.
YOKOKAWA, Prof. Toshio, Faculty of Science, Hokkaido University, Sapporo.
YOKOTA, Prof. Isaaki, Department of Physics, Niigata University, Ikarashi, Niigata.
YOKOTA, Prof. Mario, Department of Applied Physics, Osaka City University, Sumiyoshi-ku, Osaka.

YONEZAWA, Dr. Fumiko, Department of Applied Physics, Faculty of Science, Tokyo Institute of Technology, Meguro-ku, Tokyo.
YOSHIDA, Mr. Akihiko, Department of Applied Physics, Osaka City University, Sumiyoshi-ku, Osaka.
YOSHIDA, Dr. Takeshi, Department of Physics, Faculty of Science, Kyushu University, Fukuoka.
YOSHIOKA, Prof. Tatsuo, Miyagi University of Education, Aramaki Aoba, Sendai.

MEXICO

HELMAN, Prof. J. S., E.S.F.M., Instituto Politecnico Nacional, Unidad de Zacatenco, Ed. 6, Mexico 14, D.F.

NETHERLANDS

VAN DER LUGT, Dr. W., Solid State Physics Laboratory, Melkweg 1, Groningen.

RUMANIA

DRAGOMIR, Dr. Ioan, Institutul Politechnic, Faculatatea de Metalurgie, Str. Polizu 1, Bucuresti.

SWEDEN

JOHANSSON, Dr. G. A., Department of Inorganic Chemistry, Royal Institute of Technology, S 100 44, Stockholm 70.

SWITZERLAND

GÜNTHERODT, Dr. H. T., Laboratorium für Festkörperphysik, Honggerberg, CH-8049, Zürich.

THAILAND

SAMATHIYAKANIT, Dr. V., Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok 5.

UNITED KINGDOM

CROXTON, Dr. C. A., Cavendish Laboratory, University of Cambridge.
CUSACK, Prof. N. E., School of Mathematics and Physics, University of East Anglia, Norwich NOR 88C.
DAVIES, Dr. H., Department of Metallurgy, University of Sheffield, St. George's Square, Sheffield S1 3JD.
ENDERBY, Prof. J. E., Department of Physics, The University, Leicester LE1 7RH.
EVANS, Dr. R., H. H. Wills Physics Laboratory, Bristol BS8 1TL.
FABER, Dr. T. E., Cavendish Laboratory, Free School Lane, Cambridge CB2 3RQ.
FINNEY, Dr. J. L., Crystallography Department, Birkbeck College, Malet Street, London WC1E 7HX.
GREENWOOD, Dr. D. A., H. H. Wills Laboratory, Bristol University, Tyndall Avenue, Bristol BS8 1TL.
HOWE, Dr. R. A., Department of Physics, University of Leicester, Leicester.
KENDALL, Dr. P. W., International Research & Development Co. Ltd., Fossway, Newcastle upon Tyne.
MARCH, Prof. N. H., Department of Physics, The University, Sheffield S10 2TN.
NORRIS, Dr. C. A., Department of Physics, University of Leicester, University Road, Leicester.
ROSS, Dr. R. G., School of Mathematics and Physics, University of East Anglia, University Village, Norwich NOR 88C.
SEYMOUR, Prof. E. F. W., Department of Physics, The University of Warwick, Coventry CV4 7AL.
STYLES, Dr. G. A., Department of Physics, The University of Warwick, Coventry CV4 7AL.
THOULESS, Prof. D. J., Department of Mathematics and Physics, University of Birmingham, P.O. Box 363, Edgbaston, Birmingham B15 2TT.
ZIMAN, Prof. J. M., H. H. Wills Physics Laboratory, Royal Fort, Tyndall Avenue, Bristol BS8 1TL.

UNITED STATES OF AMERICA

ASHCROFT, Prof. N. W., Laboratory of Atomic and Solid State Physics, Cornell University, Clark Hall, Ithaca, N.Y. 14850.

CHEN, Dr. S. H., Nuclear Engineering Department, Massachusetts Institute of Technology, Cambridge, Mass. 02139.

KIRKPATRICK, Dr. E. S., IBM Research Center, Yorktown Heights, N.Y. 10598.

HALDER, Prof. N. C., Department of Physics, State University of New York, Albany, N.Y.

NACHTRIEB, Prof. N. H., Department of Chemistry, The University of Chicago, Chicago, Illinois.

THOMPSON, Prof. J., Physics 210, University of Texas, Austin, Texas 78712.

WARREN, Dr. W., Bell Laboratories, Inc., Murray Hill, New Jersey 07974.

WITTENBERG, Dr. L. J., Monsanto Research Corporation, P.O. Box 32, Miamisburg, Ohio 45342.

Foreword

What Do We Not Yet Understand About Liquid Metals?

J. M. ZIMAN
H. H. Wills Physics Laboratory, University of Bristol

The six years that have passed between the Brookhaven and Tokyo Conferences have allowed time for genuine development of our understanding of the nature and properties of liquid metals. The work presented at the Second International Conference and published in these Conference Proceedings should demonstrate a real step forward.

It would be impossible—and impertinent—to attempt to summarise, in a few words, all that has happened in between, or to assess the scientific status of many pieces of research that are being presented for the first time in Tokyo: that will be a task for the months and years ahead. But it may be instructive, both to the novice and to the veteran in this field, to look back at the state of the subject as it might have seemed at the end of the Brookhaven meeting, and with the benefit of a little hindsight to pick out the problems that still seem interesting. This should help us to ask the correct questions now, and to check that important issues have not been ignored.

To avoid invidious comparisons, and to keep this commentary within reasonable bounds, I shall talk in general, without reference to individuals and without citations. Let us think of this work as a collective enterprise, in which a large number of us cooperate to discover the facts and their most likely interpretation. For the details, the reader will no doubt turn to the Brookhaven Proceedings, or to his own personal collection of more recent references and data.

Let us start with a simple, well-understood point—the electronic transport properties of the alkali metals. Within the usual errors and uncertainties of theoretical physics, the nearly-free-electron formula had been shown to agree fairly well with experiment, although minor variations in the estimation of the pseudopotentials could produce large variations in the calculated transport properties. But there was still a need to stabilize these calculations, and to get much better quantitative estimates for derivative parameters such as the thermopower, and temperature and volume coefficients of resistance. Discrepancies between theory and experiment were more obvious in the ' simple ' polyvalent metals, where the thermopower would usually turn up with the wrong magnitude, if not the wrong sign. The properties of Hg seemed especially difficult to interpret, particularly when alloyed with other metals.

Nevertheless, all this seemed a routine operation of merely improving the ingredients in the formula. What was not stated at Brookhaven was that the experimental data were very incomplete, and referred almost entirely to metals of relatively low melting point. More recent measurements of the resistivity of more refractory elements such as the alkaline earths do not fit in at all well with simple pseudopotential theory: ten-fold discrepancies between theory and experiment have been disclosed.

Again, the properties of liquid transition metals were ignored at Brookhaven, except for some mysterious susceptibility data. It is true that resistivity values were available from much older work, but the theory of these was not discussed.

Since that time, some remarkable trends have been observed in the transport coefficients for this whole group, which require qualitative and quantitative explanation. It is worth mentioning, incidentally, that a good theory of the properties of liquid Fe at extreme pressures and temperatures would be a valuable contribution to geophysics, to put genuine numbers into the dynamo model for the magnetism of the earth.

We see, therefore, that the critics of the simple NFE model of liquid metals had a better cause than the possible discrepancies that they were looking for in the alkali group. What mechanisms might be invoked to explain the anomalies? Three different types of explanation seemed plausible at the time.

Was it all due, for example, to ' failure of the Born Approximation '. This is easy to say, but difficult to prove. The NFE formula is obviously suspect as merely the first term of an infinite perturbation expansion. It is natural to suppose that higher-order terms, involving the higher-order atomic correlation functions, could give rise to large corrections, although very little precise evidence for the nature and magnitude of these terms was actually given at Brookhaven.

An obvious need, therefore, was to develop an ' exact ' formula for the transport coefficients in a disordered system, not dependent on the Born approximation for the scattering factors. This means some fairly heavy analytical theory, starting off from an exact abstract expression such as the Kubo formalisms. Despite its difficulty, this is at least a genuine mathematical problem, capable of precise formulation. In particular, there was—and remains—a need for a new derivation of the Hall coefficient. This is a formidable technical problem, since the NFE approximation always gives exactly $-1/nec$ whatever the nature of the scattering mechanism. Theoretical speculation is not aided by the fact that the experimental value is often very close to this number for most liquid metals, and yet can actually become positive in a few cases.

Another obvious point of attack was on the pseudopotential or model potential used in calculating atomic form factors. Variations in this factor can cause big differences in the transport coefficients. The NFE formula is particularly vulnerable to small changes in the pseudopotential near $2K_F$, since it is the backward scattering that dominates the electrical resistivity. The energy dependence of the pseudopotential can be very important in calculations of the thermopower or the volume dependence of the transport coefficients.

This is why the resonances in atomic potentials need careful consideration. At the time of the Brookhaven conference, it was just beginning to be recognized that the *d*-band in a transition metal could be thought of as deriving from a *d*-resonance in the pseudo-atoms or muffin-tin potentials of the assembly, but this was not taken into account in any of the theories of liquid metals presented at that meeting, and there was no suggestion that similar resonances, above or below the Fermi level, might play an important part in atomic form factors in other metals.

It is surprising, also, to notice how little attention was paid to the other standard model of the electronic structure of transition metals. Only one paper at Brookhaven discussed the problem of setting up a tight-binding formalism for the *d*-electrons in a liquid transition metal. This, surely would be the natural first step to a derivation of the transport properties in terms of conduction by *s*-electrons with scattering into empty states in the *d*-band, *s-d* hybridization, etc. It would be interesting to see whether a 2-band model of a liquid transition metal could be made to work when each band must have its own spherical Fermi surface.

This thought leads to the third suggested explanation for the discrepancies now observed between experimental fact and the NFE theory. Are these

discrepancies due to the appearance of strong ' band-structure ' in the density of states? It had been established that minor variations from the free electron density of states would not give rise to changes in the calculated transport coefficients, but if there were pseudo-gaps with low energy density then localized states, or mobility edges might be expected to occur. The question was, however, how to test this experimentally. Many phenomena, such as optical absorption, the Knight shift, and positron annihilation, obviously depend on the density of states; but the evidence from these has always been somewhat ambiguous, because of uncertain factors such as matrix elements.

The calculation of the density of states from first principles is thus a clear aim of current theory. The standard perturbation scheme for such a calculation, involving atomic potentials and liquid structure factors, was already well known at Brookhaven, but the formulae had not been evaluated. Despite some substantial and reliable calculations since then, it is not certain that this sort of perturbation series is the best available method, and several other general schemes have been proposed. In all this, the effect of the disordered structure may be less important than the nature of the atomic potential. For example, a *d*-resonance should show up clearly as a strong *d*-band hump in the density of states, whatever the arrangement of atoms. We might ask, similarly, whether some other feature of the local potential can give rise to pseudo-gaps in appropriate circumstances.

What was, I think fairly well established at Brookhaven was that the structure factor itself plays a relatively passive role in the theory of the electronic transport coefficients. It can be measured with greater accuracy than the other factors in the NFE formula, and is much the same for most pure liquid metals. But we need a good theory of this fundamental function, especially if we are to predict its form under extreme conditions such as high temperatures and pressures.

At Brookhaven, there were two firms active in this conventional large-scale industry. One approach was through molecular dynamics, using real-space, real-time, Monte-Carlo models. The competing method was to try to solve analytically the hierarchy of equations for the atomic correlation functions. It was satisfying to observe that both methods were getting quite good results, in adequate agreement with experiment.

The more interesting question was whether the details of the radial distribution function in a liquid can provide reliable evidence about the nature of the interatomic forces. Was it really true that these forces, in metals, have relatively long range oscillatory terms, associated with Friedel oscillations in the screening charges? The question was then left open: what is the present position concerning this fundamental physical parameter?

From there we go on to the study of the dynamics of liquids. Plenty of data from inelastic neutron diffraction have now been available for some years, but a complete quantitative analysis of the collective and particulate motion in liquids was still lacking. This branch of the subject is not necessarily confined to metallic liquids, but these provide good experimental test materials for models of spherically symmetrical monatomic fluid systems.

Inelastic neutron diffraction is an expensive and somewhat contrived phenomenon to observe: atomic diffusion in liquids is a significant macroscopic parameter of great practical importance under quite simple physical conditions. At Brookhaven, only empirical correlations were noted, and the models used for theoretical derivation of diffusion coefficients were obviously inadequate. One puzzling phenomenon did, however, get a good quantitative explanation. The electromigration of impurities in liquid metal solvents was shown to be due to momentum transfer from the current of conduction electrons, and thus depends mainly on the differential resistivity of solvent and solute species.

We now come to the study of the electrical properties of liquid alloys. In many ways, these are subject to the same theoretical principles as the pure liquid metals. To calculate the transport coefficients, one only needs structure factors and pseudopotentials. But the experimental data are much richer, and the sources of uncertainty or error are that much greater—with all that this implies by way of speculative conjectures, adjustable parameters and fudge factors. At Brookhaven the characteristic puzzles and theoretical possibilities were already beginning to show up. It was obvious, for example, that information about partial structure factors was essential, either through sophisticated experimental research or by inspired theory. The time has come to give analytical meaning to terms like ' clustering ', ' bonding ', ' local order ' which have been used rather loosely and qualitatively in the past and to derive the appropriate statistical distribution functions directly from the interatomic forces, with due deference to the geometrical constraints. Are the vagaries of the partial structure factors responsible, for example, for the mysterious behaviour of the alloys of Hg, which was vaguely attributed to ' band structure effects ', or is this due simply to resonances in the atomic pseudopotentials? As for the Hall effect, susceptibility Knight shift, etc., etc., in liquid alloys, there is much qualitative speculation but almost nothing quantitative in the Brookhaven proceedings.

Nevertheless, we must be very careful not to avoid the really important problems just because they are practically unsolved. Such basic thermodynamic parameters as the partial enthalpy of mixing of liquid metals can often be described phenomenologically with parametrized formulae, but there is no theory for the deviations from ideal solution behaviour. Explanations of excess volume of mixing are quite lacking. It is useless to turn to the corresponding data for solid alloy phases, since these are even more difficult to understand. Indeed, the liquid alloys are the simplest metallic mixtures and should be studied with all the forces that we can muster—experiments on photo-emission, soft-X-rays, partial structure factors, etc., associated with theories of ineratomic forces, electron charge distribution, and so on. Scientific mastery of the energetics of liquid alloys is one of the most important goals of our research.

Another modification of a pure liquid metal is obtained by expanding it, above its critical point, into a low density fluid or vapour. In addition to its interest from a thermodynamical and statistical point of view, this phase shows remarkable electrical behaviour. The transition from a metallic to a semiconducting regime was reported at Brookhaven, but the mechanism of this transition has not been proved decisively. It may be due, for example, to the appearance of a pseudogap containing localized states, due to the increase of disorder. Or it may be a cooperative transition of the electron distribution, going over from a nearly-free-electron gas, with long range screening of ionic charges, to localized electrons on the atom and molecules. Another theoretical possibility is a percolation transition associated with the absence of continuous paths along which electrons can move from atom to atom. We must hope to get better evidence for and against these various hypothetical mechanisms—although the true situation may only be describable in terms of all three effects acting simultaneously. It is interesting, also to speculate on whether the mutual interdependence of electron–electron screening and interatomic forces can actually drive the thermodynamic critical point into synchronism with the metal-non-metal transition.

It is helpful to study the chemical analogue of a dense metal vapour—the metal-ammonia solutions, which certainly show a rapid transition to metallic conduction at sufficiently high concentrations. The thermopower also goes over very convincingly from semiconductor to metal values. The experiments on

these systems are by no means new, but they certainly deserve continued research and careful theoretical analysis.

Another analogue of a metallic vapour is impurity-band conduction in doped semiconductors. But this system is really much more complex because the impurities themselves can be of opposite signs (i.e. partially compensated). From the point of view of a mobile carrier, it is also significant that many pairs of neighbouring impurities may lie much closer together than the characteristic Bohr radius of an impurity level wave function. This model is therefore much more like a gas than a liquid.

Finally, experiment and theory is being extended to liquids that one would expect to be metallic, and which yet seem more like semiconductors in their electrical properties. The most extraordinary case is the alloy of Mg with Bi. Both Mg and Bi make perfectly good NFE liquid metals; yet in the neighbourhood of the concentration 60% Mg, 40% Bi the liquid mixture has quite a low conductivity. More such cases have now been studied and present a real challenge to theory. Is this again a structural effect, where Mg_3Bi_2 molecular complexes form temporarily in the liquid, or is it something to do with electron transfer to produce an 'ionic salt' containing Mg^{++} and Bi^{---} ions? Another example is the range of behaviour of the Se–Te alloys, which varies from metallic liquid Te to semiconducting liquid Se. What is the essential difference between these two elements in the liquid state?

From this point we could go on to discuss the unusual properties of amorphous and glassy semiconductors. The fundamental question, which was asked in 1966 but which is still not adequately answered, is how we can get band gaps in a material without long range order. But this is a good enough problem for a theoretical conference of its own: we must somewhere draw a line about our subject.

I have tried here to show the general nature of the problems in this field, as they might have seemed five or six years ago. The question we must ask, after attending the Tokyo Conference or reading these Proceedings, is how much further progress we have made. I think that some problems will now look very simple and may be judged solved in principle. Other problems may seem less interesting, quantitative calculations being dependent on too many uncertain parameters to be worth lengthy computation. But I guess that the field of research into liquid metals will remain for some years in a healthy state, with many difficult experiments and speculative theories to keep us all happy.