

Summary

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Summary

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I have been given the task of summarizing the achievements of the Oji Seminar on the 'Quest for New Physical Phases under Extreme Conditions'. This is an enormous task and I consider it as impossible to attempt to summarize, in a few words, the status of a seminar which is, itself, a reflection of a rapidly developing field which is highly active, as is obvious from the 37 lectures that were given, and from the more than 20 posters. And it is a field which is so diverse and so dynamic that within the scope of this summary it is impossible to mention all of the important recent developments, and it is even more futile to try to define emerging areas of opportunities. Recent history teaches us that new discoveries come unexpectedly as a result of excellent work by researchers, and *not* as a result of careful planning by committees or in seminar summaries. An illuminating example of this in the context of the seminar to which this Special Issue is devoted is the exciting progress in the search for metallic hydrogen. Exactly four years ago I listened during the Oji Seminar on 'Elementary Processes in Dense Plasmas' to a beautiful review lecture on the long history of searches for the metallization of solid hydrogen under static pressures at low temperatures, presented by Russel Hemley. On the basis of the experimental progress that he described, I speculated at that time that we could expect solid hydrogen to become an alkali metal within five to ten years. But despite an unrelenting experimental assault at pressures up to 340 GPa (Narayana *et al* 1998), dense solid hydrogen has so far defied all attempts at metallization. The actual experimental status at the time of the present seminar was critically analysed in the pedagogically beautiful lectures of Russel Hemley and Isaac Silvera. They emphasized that to date, most probes of a possible metallic state have been optical, and for sceptics the only rigorous criterion for differentiating between a metal and a nonmetal is to measure the static conductivity.

Ironically, it was a high-temperature experiment on shock-compressed fluid hydrogen which first claimed to metallize hydrogen in the (disordered) fluid state at pressures for which the (periodic) solid is still in the insulating phase. The discussion of this experiment following the lecture of Weir clearly demonstrated that this new fluid state of hydrogen raises basic questions of definition. There is no clear dividing line between metals and nonmetals. The Livermore data clearly reveal a dramatic increase in the electrical conductivity of fluid hydrogen under pressure, reaching a limiting value of approximately $2000 \Omega^{-1} \text{ cm}^{-1}$, i.e. a value which is comparable with those for expanded liquid alkali metals in the density region where metallic properties evolve continuously into those characteristic of nonmetals. Importantly, this measured conductivity is comparable to that calculated on the basis of the assumption—reported by Ioffe, Regel, and Mott—that high-temperature fluids only metallize, and remain metallic, when the mean free path of the valence (conduction)

electrons becomes comparable to, or exceeds, the mean distance between the particles supplying the electrons.

Various other approximate criteria exist for defining a boundary between metal and nonmetal but there is no rigorous definition valid for a fluid at high temperatures. The only rigorous criterion for differentiating between a metal and a nonmetal is the electrical conductivity at the absolute zero of temperature; there, metals have a finite conductivity (with the exception of superconductors, which show infinite conductivity), whilst nonmetals have zero electrical conductivity. At any nonzero temperature, however, thermal excitation of conduction electrons, no matter how few, blurs the difference between the metal and nonmetal. Yet only the most rigid purist would seriously question the designation of liquid sodium as a metal at its melting point. The properties of this liquid are, for all practical purposes, very similar to those of an ideal metal. Thus there is general agreement on calling fluid alkali metals just metals. Be that as it may, there is no doubt that at high temperatures and in the pressure range above 140 GPa fluid hydrogen becomes highly conducting. The importance of this result for planetary modelling, in particular for defining the zone of possible dynamo generation, was emphasized in the lecture of Stevenson. A conductivity close to the Mott–Ioffe–Regel value is more than enough for that purpose.

Much progress has been made in understanding the recalcitrance of solid hydrogen as regards metallization. Ashcroft described in his lecture a remarkable spontaneous electronic polarization of hydrogen dimer molecules at ultrahigh pressures. In clear contrast to the normal-pressure situation, in which a hydrogen molecule has precisely equivalent charge density at both protons, at high pressures the electronic charge piles up preferentially at just one of the constituent protons. The hydrogen molecule thus develops a permanent electric dipole moment. The presence of this partially ionic character in the ground state of dense solid hydrogen may serve to delay the long-awaited transition to the metallic state. The Ashcroft calculations suggest that a band-overlapping metal could appear at about 350 GPa which is followed by a transition to a monatomic phase which may occur at pressures typified by 400 GPa.

Hydrogen is not the only material in which the electronic structure depends strongly on the thermodynamic state. Amaya's group from Osaka University has pioneered the development of ultrasensitive electrical and magnetic techniques and tested them on a long list of materials under pressure. An impressive number of solids that are electrical conductors at atmospheric pressure have been made metallic and superconducting at high pressure. Courageous theorists like Nagara, Tsumeyuki, and Miyaga are willing to predict not only the structures of solid hydrogen, but also those of the halogens and other elements at megapressures.

It goes without saying that planetary modelling poses additional fascinating questions that can be addressed by high-pressure research. A 'wish list' of experiments and theory needed to make further advances was presented in the lectures of Stevenson, Chabrier, Winget, Isern, and Yoshida. To the group of important unresolved issues belongs the behaviour of hydrogen, including the possible existence of an abrupt plasma phase transition, at the high pressures and temperatures prevailing in the giant-planet interiors.

The path-integral Monte Carlo study of isochoric heating of dense hydrogen presented by Ceperley seems to be an interesting attempt to improve our quantitative knowledge of the phase diagram of hydrogen. Unfortunately in this work the electrical conductivity was not reported. In the seminar, because of the interest in the states of matter in massive planets and brown dwarf stars, the relation of the Ceperley computer experiment to the work of Chabrier is of relevance. As Chabrier emphasized, on the basis of chemical considerations, the most striking feature is that molecular dissociation and pressure ionization occur at almost the

same density at any temperature. Pressure ionization does not occur after dissociation of all molecules in atomic hydrogen, but rather directly from the dense molecular fluid. Atomic hydrogen plays a minor role in pressure ionization within Chabrier's chemical approach. In the Ceperley experiment, dense hydrogen has been simulated starting from an assembly of fully interacting protons and electrons. He finds that the molecular dissociation transformation occurs at somewhat lower temperatures than given by the chemical approaches. A noteworthy observation is that at high density the dissociation process is accompanied by decreasing pressure, which is interpreted as an indication of a first-order transition. Ceperley stressed the similarity with the so-called plasma phase transition exposed by the chemical model of Chabrier. In both cases the phase boundary has a negative slope which is interpreted as being due to the cooperation of temperature and degeneracy in dissociation.

It was emphasized by Stevenson and Chabrier that the nature and the location of this transition is highly relevant to any discussion of the way in which giant planets and brown dwarfs evolve. This all has implications affecting their atmospheric abundances, in addition to the proposed limited solubility of helium, water, methane, etc in metallic hydrogen.

It is self-evident that laboratory studies designed to clarify the heterogeneous phase equilibria of fluid mixtures at high pressures will be required before detailed models can be constructed. The most pressing need is for high-pressure data on mixtures of helium. Unfortunately, until now it has not been possible to investigate the phase behaviour of these mixtures at the extreme conditions where hydrogen becomes metallic. In the light of the unfavourable outlook for such measurements, effort has been spent on investigating phase diagrams of systems which might serve as models for the hydrogen–helium system. Of special interest in this respect is the mercury–helium system, because mercury has a liquid–vapour critical point and a metal–nonmetal transition density which lie within the range of experimentally accessible conditions. Although the characteristic metal–nonmetal transition densities for metals are considerably less than those for hydrogen, the fluids themselves are expected to be very similar in their behaviour, as discussed in the lectures of Tamura and Hensel. Thermal ionization, formation of chemical species, and strong electron–electron interactions are only a few of the phenomena that play important roles in the metal–nonmetal transitions in fluid metals as well as in fluid hydrogen. The metals may therefore serve as working models for the metallization of fluid hydrogen.

Strong dependence of the electronic structure on the thermodynamic state implies a corresponding variation in the nature of the interparticle interaction in any fluid system. How difficult it is to understand radical changes in electronic structure and their implications for the interactions between particles in the fluid became obvious from the theoretical contributions of Yonezawa and Hoshino on elemental fluid selenium, which undergoes a metal–nonmetal transition that involves changes in both density and temperature.

Another topic which clearly demonstrated that many physical questions related to the metal–nonmetal transition in disordered systems are common to solid and fluid systems was that of strongly correlated electrons and 'high-temperature' superconductivity. Studies of the transition range of expanded fluid caesium, for example, reveal electron–electron correlation effects that are related to the magnetic properties of 'high-temperature' superconductors. We learned from the lecture of Liang, who presented an impressive collection of experimental data, that these are systems with unusual electronic structure. Again, there seems to be support from an examination of the normal-state transport properties of systems undergoing composition-induced changes in the electronic structure that the nonmetal–metal crossover is intimately linked to high-temperature superconductivity. Important advances in the understanding of this link from new theoretical views of high-temperature superconductivity

were presented by Kamimura and Nagaosa.

One of the most exciting sessions of the seminar was that devoted to the study of phase transitions under strong magnetic fields. The significant progress in our understanding of various physical processes responsible for neutron star cooling was discussed in the lecture of Salpeter. He studied the physical properties of different hydrogen phases on the surface of a strongly magnetized neutron star for a wide range of magnetic field strengths B and surface temperatures T . Depending on the values of B and T , the outer envelope can be either in a non-degenerate vapour phase or in a degenerate metallic phase. For high enough field strength ($B \geq 10^{13}$ G) there exists a first-order phase transition from the non-degenerate vapour phase to the condensed metallic phase.

Ultrahigh magnetic fields up to several megagauss—now available in the laboratory—can be used to induce fundamental changes in the character of an electronic system. Interesting phenomena related to the effect of these high magnetic fields on the metal–insulator transition have been discussed in the lectures of Miura and Takada. An electronic transition in graphite is interpreted as a manifestation of a nesting-type instability inherent to a one-dimensional narrow Landau sub-band. A nice pedagogical introduction to the field-induced spin-density waves found in organic conductors of the Bechgaard type, along with experimental results on related high-magnetic-field phenomena, was presented by Chaikin. From there, the seminar went on to the study of the effects of magnetic fields on quantum wells and superlattices in the lecture of Nicholas and on the Anderson transition in the lecture of Ohtsuki.

The diversity of disciplines that were represented by the participants in this Oji Seminar became particularly obvious in the session on complex systems under extreme conditions. The lecture of Iyetomi clearly demonstrated that the quest for new physical phases can profit from deeper insight into the interrelation between superionic conductivity and electronic properties of a solid electrolyte. Ogata showed that the study of the physics and chemistry of metal clusters provides extremely valuable opportunities to explore the properties of matter in aggregates intermediate between the molecular and condensed phases. Of special interest also are polar fluids. Many of them are of considerable technical importance because of their solvent properties, often exhibited under unusual conditions of density and temperature as discussed for the case of water in the contribution by Yao. Much progress has been made in characterizing the phase behaviour of fluids in the vicinity of a substrate. Dietrich convincingly demonstrated that spatial confinement and wedge wetting are other examples for fluids under extreme conditions. Other examples of phases under extreme conditions are systems far from equilibrium. The effects of shear flow and the nature of metastable systems have been discussed in the lecture of Onuki, and the structure of and relaxation in glasses in the lecture of Odagaki.

Finally, there were two lectures by Goldstein and Winter on biorelated fields. One may ask what the current connection is between biorelated fields and new phases under extreme conditions. The two lectures nicely showed that the answer is not simply the routine application of available technology to biological systems. The structure, dynamics, and shape transformation of biomembranes present fundamental and new questions that require the insights of and creativity in physical chemistry. We learned that there are also technological opportunities. One aim is to develop a scientific food engineering basis for design, evaluation, and optimization of combined high-pressure/temperature processes to permit industrial application.

It is my impression that it was a very interesting week in Tomakomai. I think that after that week some ‘New Physical Phases’ look very simple and may be judged as understood. But it is evident that we are still far from understanding many of the important phenomena

which were discussed during the five days of this seminar. I think that the field of research into planetary modelling will remain in an active state for many years. The search for condensed matter properties which may be of interest for this modelling will continue. In particular, the search for an answer to the question of whether the plasma phase transition is real or not will continue to be a challenge. The solubility of helium in metallic hydrogen is still not well understood.

Finally, we owe a collective debt of gratitude to Professor Itoh for having provided—in a period which becomes more difficult for science in Japan—very good conditions for this seminar. I wish to thank him also for his scientific contribution on high-temperature plasmas in clusters of galaxies. His exact calculations which took relativistic effects into account provide important results for astronomy and may help to determine the age of the Universe. Last but not least, we thank in particular The Japan Society for the Promotion of Science and the Fujihara Foundation of Science for supporting the seminar.

Reference

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