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THEORETICAL STUDIES OF ELECTRON CONDUCTION THROUGH  
ATTACHING GASES(U) PITTSBURGH UNIV PA DEPT OF PHYSICS  
J N BARDSLEY 31 MAY 83 N00014-82-C-0021

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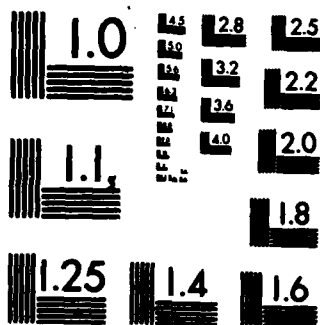
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The motion of electrons in gases containing a mixture of moderating and attaching molecules is explored through Monte Carlo simulations. The results are used to check analytic theories based on the Boltzmann equation. Applications are made to transient problems associated with the pulsed power program. The possibility of fast operation of a diffuse discharge opening switch has been demonstrated, through the study of simple models. More detailed analyses of spatial and temporal inhomogeneities are underway. The basic atomic physics data necessary for these studies are obtained by semi-empirical calculations. Analyses of laboratory measurements.		

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## Interim Report\*

ONR Contract N0014-82-0021

with The University of Pittsburgh

## "Theoretical Studies of Electron Conduction Through Attaching Gases"

Period covered: July 1, 1982 - May 31, 1983

1. Principal Investigator: J. N. Bardsley, Professor of Physics
2. Contract Description: To perform theoretical studies of the motion of electrons through gas mixtures, containing some molecules which easily attach electrons and others that are efficient energy absorbers, in order to provide information about the conduction of electrons in gas discharges. Particular attention will be given to those discharges which are suitable for optically controlled switches or other similar devices being developed in the DOD pulsed power program.
3. Scientific Problem: a) The major goal is to identify a gas mixture with two phases, one of low electrical resistivity and the other of high resistivity which can be changed rapidly from one phase to the other. The transition could be achieved electrically through changes in the applied voltage, or optically through irradiation by laser light. Such a gas might form the active medium in a diffuse discharge switch that could operate without the movement of electrodes or the addition of large amounts of gas during the opening of the switch.
4. Scientific and Technical Approach:
  - a) A Monte Carlo simulation code is being developed to permit modelling of arbitrary mixtures in both time-independent and time-dependent situations. The model can incorporate the spatial characteristics of specific devices, but will be first used in simple analyses of homogeneous discharges.
  - b) The theory of the transport of charged particles through molecular gases is being developed to take account of transient phenomena and spatial inhomogeneities that may be important in pulsed-power applications.
  - c) The Monte Carlo code will be used to check the accuracy of the transport theory and to resolve any discrepancies that may appear between the results of differing theories.
  - d) The influence of high gas densities upon atomic reactions will be studied. This is necessary because many two-body reactions are enhanced by the ambient gas molecules, whereas three-body processes can saturate as the density is increased. These effects are particularly important for recombination and attachment reactions.

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e) The characteristics necessary for rapid opening of a switch will be identified and several candidate systems will be selected. The merits of these systems in the conduction phase will then be tested.

This work will be performed in conjunction with the studies being carried out in the Electrical Engineering Department at Texas Technical University. The main contacts with that group are Professors Kunhardt, Schaeffer and Schoenbach.

#### 5. Progress:

a) The Monte Carlo program has been applied to several systems in a variety of situations, including  $N_2$ , Ne and Ar as the buffer gas,  $N_2$ , NO,  $CO_2$ ,  $NH_3$  as the moderator (energy absorber) and HCl,  $NF_3$  and  $N_2O$  as the electron attacher.

b) A mass-scaling technique has been developed that increases the efficiency of simulations in dilute mixtures of molecular gases in a rare-gas buffer by several orders of magnitude. The method has been applied to mixtures of NO and Ar, to assist in the interpretation of recent afterglow measurements.

c) It has been demonstrated that very small amounts of attaching molecules like  $NF_3$  or  $N_2O$  in  $N_2$  near atmospheric pressure can remove most of the electrons in a discharge in a very short time. The non-adiabatic effects associated with the growth of the electric field during the opening of a switch are small at such pressures with nanosecond rise times.

d) The measurements of attachment rates in pure HCl and in dilute HCl- $N_2$  mixtures have been shown to be consistent. The five-fold difference in the measured attachment rates arises from the different speed distributions in the two experiments. In pure HCl, the speed distribution is much broader than the expected Maxwell-Boltzmann distribution, and evidence is seen of "hole-burning" near the peak of the attachment cross section.

e) Significant differences have been found in the longitudinal diffusion coefficient as computed by various authors. We have identified and corrected one error made by several authors in the application of the free-path method. However, there still remains an uncertainty regarding the comparison of Monte-Carlo results with those of Pitchford and Phelps using the density gradient expansion method.

f) In order to examine the validity of the density gradient expansion, we are studying the higher order diffusion coefficients, which control the deviations from the simple Fick's law. These deviations have been observed in recent studies of arrival-time spectra of ions in drift tubes. Application to a simple model seems to show a discrepancy between the results of the free-path and Monte Carlo methods and those of the density gradient approach to the solution of the Boltzmann equation. This will be investigated further.

g) The principal investigator participated in a workshop on repetitive switches at Tamarron in which the characteristics of a diffuse discharge closing switch were developed as an alternative to the magnetic switches currently being developed. The design made use of much of the basic physics learned during the opening switch research program.

## 6. Publications:

- a) Dissociative Attachment in  $\text{HC}_2$ ,  $\text{DC}_2$  and  $\text{F}_2$ , J. N. Bardsley and J. M. Wadehra, to be published in J. Chem. Phys. (1983).
- b) Monte Carlo Studies of Attachment in  $\text{HC}_2$  and  $\text{HC}_2$ -  $\text{N}_2$  mixtures, B. M. Penetrante and J. N. Bardsley, submitted to J. Appl. Phys.

## 7. Extenuating Circumstances: None

8. Unspent Funds: Very little funds will remain unspent as of September 30, 1982, assuming that the anticipated delivery of computing equipment is not unduly delayed.

9. No students have graduated during this period. B. M. Penetrante's thesis overview has been endorsed by his Ph.D. committee.



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