METASTABLE ENHANCEMENT OF C^+ AND O^+ CAPTURE REACTIONS

FINAL REPORT

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I INTRODUCTION

The project is devoted to the study of charge transfer neutralization of Carbon and Oxygen ions in H and H_2 gases at energies from 10 to 500 eV. A major motivation was to provide cross section data to support analysis of edge plasmas in Tokamak Fusion devices.

The first objective was to measure cross sections for metastable excited singly charged ions separately from the cross sections for ground state ions. Previously published values are confusing because the beams used included unknown fractions of metastables and these metastables have cross sections greatly different from the ground states. The program was fully accomplished, metastable cross sections were found to be over an order of magnitude greater than the ground state and existing discrepancies in the literature were resolved. Considerable effort was devoted to the design and operation of ion source configurations were the metastable content of the ion beam was known.

Subsequently we have moved to study neutralization of multiply charged C and O ions in the same targets. First there has been a need to develop ion sources which can produce useful beams of multiply charged species. This has now been accomplished. The intent is to use these sources for the measurement of cross sections with again an attempt to differentiate between the behavior of ground and metastably excited species.

II PROGRESS OF THE WORK

As the project proceeded the results were rather frequently and fully published in the open literature. To summarize the results and progress we shall largely confine ourselves to the reproduction of the abstracts of these publications.

The majority of the published work relates to the study of metastable ion neutralization. The basic detection technique was to study the attenuation of the ion beam as it traversed a target gas cell. The attenuation can be related to gas pressure, cell thickness and the cross section for charge transfer neutralization. If two species are present (e.g. metastable and ground state) which exhibit greatly different cross sections then the attenuation curve can be deconvoluted to give the two separate cross sections. The deconvolution procedure also allows one to measure the metastable content of the ion beam as a ratio to the total beam. As a source of ions we used an electron impact source where the electron energy could be rather closely controlled. Thus by selecting an electron energy below the threshold for metastable ion production but above the ground state ionization threshold one may produce beams for only ground state species. These can be used for a ground state measurement free of any confusion about the presence of metastables. At higher electron energies one may produce both metastable and ground state species for which the separate cross sections may be evaluated by the attenuation deconvolution. With the information on the ground state alone one can separate identify the metastable behavior. We should perhaps note in passing that the flight length of the apparatus was sufficient that any excited states that radiatively couple to the ground (or metastable) states will decay before the ion beam enters the collision region.

We discussed our studies of charges transfer neutralization of oxygen ions in a paper with the following abstract (1):

> Cross sections for charge transfer reactions of ground $O^+(^4S)$ and metastable $O^+(^2D,^2P)$ state ions with H_2 have been measured for reactant ions with 10 to 500 eV kinetic energies. Ground-state ion cross sections range from 0.5 to 0.9×10^{-16} cm^2 and metastable-state ion cross sections are approximately constant at 10×10^{-16} cm^2.

A similar paper with full experimental details contained our data on the neutralization of the carbon ions and had the following abstract (2):

> Cross sections for charge-transfer reactions of ground-state $C^+(^2P)$ and metastable-state $C^+(^4P)$ ions with H_2 have been measured in the 10-to 500-eV kinetic energy range. Ground-state reaction cross sections range from 0.3 to 0.5×10^{-16} cm^2, and the corresponding values for metastable state $C^+(^4P)$ ions vary from 20 to 12×10^{-16} cm^2. Both sets of cross-section values smoothly extrapolate to previously measured data at higher energies.

Typically the cross sections for the metastable state were an order of magnitude of more higher than those of the ground state at low energies. A major result of the work was to show that previous measurements of these processes by Gilbody's group were in fact totally incorrect due to inadequate assessment of the metastable content of the ion beams they utilized. Prompted by our results Gilbody repeated most of his previous work and completely confirmed the observations of the present project.

The interest in the metastable state composition led us to perform a brief general study of what metastable carbon fluxes could be obtained from ionization of various carbon containing gases. The highest fraction was found from CO, some 32 %. Gases with CH bonds generally gave metastable fractions of about 20-25% and those with a CN bond only 15%. These fractions were obtained for electron impact ionization at 100 eV; that is far above threshold. We believe at these energies the metastable fraction is rather independent of energy and probably representative of any ion source configuration including a plasma device. The results have been fully reported in a paper with the following abstract (3):

An experimental technique has been developed to determine the fraction of metastable ions present in beams. The technique involves measurement of total electron capture cross sections from neutral species where individual ground and excited state reactant ion cross sections are known. Metastable C II ion abundances from electron impact ionization of various molecules have been obtained.

We further wished to pursue these studies by seeking the same type of cross section information for highly charged ions of O and C. We first attempted to predict what sort of metastable populations would be obtained from an ECR plasma type source utilizing a stepwise ionization model. Cross sections are based on the semiempirical model of Lotz. Comparison could be made between predictions and our own measurements as well as the measurements of other groups. Good comparisons were obtained and the results are fully published in a paper with the following abstract (4):

A simple ionization model has been used to compute metastable beam populations for atomic ions formed in low density, high electron temperature ECR plasma type ion sources. Metastable fractions for each charge state of atomic carbon, nitrogen and oxygen have been evaluated. Computed metastable fractions are found to be in reasonable agreement with experimental data.

With the prediction of source operating conditions in hand we have no turned to the design of an ECR source that will produce highly ionized ions and in particular ions of all state of C and O. The intent is that the source should be compact and readily retrofitted to existing ion accelerator systems. This has been achieved with a novel magnetic mirror structure based on permanent magnets. The design has now been submitted for publication with the following abstract (5):

A novel compact electron cyclotron resonance (ECR) ion source has been constructed and its performance characteristics evaluated using a double focusing mass spectrometer system. The source is particularly well suited for applications where beams of multiply charged ions of moderate intensities are utilized as, for example, in certain atomic physics experiments. The design features an adjustable all permanent magnetic mirror structure and a low microwave (2.45 GHz) power requirement. This low cost, simple source provides a practical alternative to larger more sophisticated ECR ion sources when production of intense beams of highly charged ions is not required. Detailed analysis of the novel magnetic structure is presented. Both charge state and kinetic energy distributions of up to eight times ionized argon as well as total extracted ion currents resulting from differing source operating parameters are given. The end loss ion temperatures for each of these argon charge states has also been determined.

ECR sources, relying on multiple electron impacts, offer the opportunity to produce molecular species not readily observed in other collisional situations. This has led us to utilized our ECR design to search for the elusive CH^{2+} ion that has sometimes been reported. Our conclusion is that the species does not exist and we have provided theoretical calculations to show that the configuration should be repulsive. The work has been submitted for publication with the following abstract (6):

> Experiments with an electron cyclotron resonance ion source have been employed in a hunt for the elusive CH^{2+} ion. Our experiments do not find evidence for the existence of stable CH^{2+} ions. Different levels of ab initio molecular orbital theory have been employed to obtain potential energy curves for CH^{2+}. Although SCF calculations show a small minimum in the potential, post-Hartree-Fock computations indicate CH^{2+} states to be repulsive.

The majority of the experiments described in our various papers involved targets of molecular hydrogen. It was, however, always our intent to perform the same experiments with an atomic hydrogen target. This was to be done with the H in the form of a beam with dissociation taking place in an RF discharge. A source was designed and reported with the following abstract (7):

> A practical technique is described to estimate the resonant frequency of a helical resonator surrounding a coaxially mounted discharge tube. A simple formula is derived that relates the resonant frequency of the cavity to dimensions and dielectric properties of the discharge tube and its contents. An experimental test is performed on a resonator used to power an RF discharge, designed to produce an atomic hydrogen beam for an atomic collision experiment. The formulation adequately predicts the resonant frequency for a helical resonator that contains a discharge tube and cooling water jacket.

Unfortunately the degree of dissociation obtained in the configuration was only about 60% with the remainder being molecular hydrogen. Moreover the collision chambers available to us were of only modest vacuum quality and exhibited significant backgrounds of H_2. Inevitably the observed signals are a mixture of signals due to neutralization in the (desired) atomic beam and in the (undesired) molecular beam or background. As a result it was not possible to separate out the atomic H cross sections and the experiment is, to date, a failure.

As a subsidiary study one of us also undertook some extensive reviews of how atomic particles interact with surfaces. The principle objectives were to collect and assess data which might be required for the modelling of Plasma Fusion devices. One paper considers how hydrogen particles reflected from materials that are candidate first wall materials for Fusion devices. That work is in publication with the following abstract (8):

> Previously published data on particle backscattering from surface under normal incidence conditions is reviewed in order to arrive at a general scaling relationship in terms of projectile energy and the masses of the colliding species. A single empirical formula is proposed which, with suitable coefficients, represents the available data base and provides a basis for interpolation and extrapolation. The formula is intended for use in codes for the modeling of particle recyclying in fusion reactor devices. Attention is focused primarily on light projectile (H, D, T, He) reflection from candidate plasma facing materials and covers an energy range from tens of eV to 100 keV to encompass situations of interest in a fusion device. We also review briefly the case of self-ion reflection.

A second paper considered the available data on electron reflection from solids and coefficients for ejection of secondary electrons. That work is also fully published with the following abstract (9):

> Particle induced electron emission from the wall of a plasma device alters the sheath potential and plasma transport in the scrape-off layer. Incident electrons eject electrons from a solid by a kinetic process. The ejected electrons cannot be distinguished from the reflected electrons and so the total yield is the sum of the two processes. Heavy particles eject electrons by the kinetic mechanism; when the projectile is ionized or excited, there may also be a contribution from potential ejection processes. Available data on electron ejection and electron reflection are reviewed, the most reliable data selected and, where appropriate, formulas are proposed that represent the functional dependence of the yield on the impact energy and impact angle.

III PUBLICATIONS

Nine major publications supported wholly or in part by the DOE have been prepared and are listed as references 1 through 9 in this report. Copies of those published have already been transmitted to DOE.

IV PERSONNEL

Principal investigator for the project was E. W. Thomas of the school of Physics. Co-PI is T. F. Moran of the School of Chemistry.

Dr. Yaodong Xu obtained a Ph.D degree based on this work. Mr. R. F. Welton will shortly write a Ph.D. thesis based on some of this work with completion projected within the next six months.

The project benefitted greatly from extensive interactions with other faculty and students at Georgia Tech particularly with R.K.Feeney of EE.

V FUTURE WORK

No further support is being provided by the DOE. It is however anticipated that the study of charge transfer neutralization of highly charge ions will continue with support from other sources.

VI FINANCIAL MATTERS

All funds are now expended and financial reports have already been submitted in the required format.

VII REFERENCES

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(8) E.W.Thomas, R.K.Janev and J. Smith. Nuclear Instruments and Methods in Physics Research B, (in course of publication).

(9) E.W.Thomas, Nuclear Fusion, Supplementary Volume 1, 79 (1991).1