Absolute cross sections for near-threshold electron-impact excitation of the $3s^2\ ^1S \rightarrow 3s3p\ ^1P$ and $3s^2\ ^1S \rightarrow 3s3p\ ^3P$ transitions in Si^{2+}

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Absolute total cross sections for electron-impact excitation of the $3s^2\ ^1S \rightarrow 3s3p\ ^3P$ and $3s^2\ ^1S \rightarrow 3s3p\ ^1P$ transitions in Si^{2+} were measured using the merged electron-ion beams energy-loss technique. The results are compared to R-matrix close-coupling theory, which predicts a strong resonance enhancement of the cross section near the threshold for excitation of the ^3P state and this is confirmed by the experiments. The observed disagreement between theory and experiment for the dipole excitation is suggested to be due to resonance interference. [S1050-2947(97)05911-8]

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I. INTRODUCTION

The description and modeling of natural and laboratory plasmas require quantitative information on the atomic processes occurring within the plasma. An important area, particularly in hot plasmas, is that of electron-ion collisions and great effort, over many years, has been applied to generating reliable cross sections for the various collision processes. The extremely large amount of data required has been, and will continue to be, provided predominantly by theoretical calculations. The role of experimenters will be to measure selected cross sections to serve as tests of the theoretical methods.

In the specific case of electron-impact excitation of multicharged ions, the calculated cross sections frequently display the presence of numerous resonances [1]. Although the influence of the resonances on rate coefficients in a plasma may be significant, particularly at low temperatures where a small number of resonances can dominate the rate coefficient, very few electron-impact excitation experiments have provided adequate tests of their theoretical description [2]. Furthermore, few nondipole excitations have been studied experimentally [3] even though resonance structure is often predicted to dominate the cross sections.

This paper represents a continuation of our program to measure excitation cross sections in ions that will provide tests of the resonance theory. Earlier measurements [4] on Kr^{6+} confirmed experimentally, the extreme sensitivity of the interference of resonances to their exact energies [5]. This conclusion was reinforced by measurements [6] on the simpler, Mg-like ion, Ar^{6+}. We are now reporting data on the excitation cross sections for the $3s^2\ ^1S \rightarrow 3s3p\ ^1P$ and $3s^2\ ^1S \rightarrow 3s3p\ ^3P$ transitions in the isoelectronic ion Si^{2+}. Strong dielectronic resonances are predicted [7,8] in the near-threshold region for the spin-forbidden transition leading to an extremely high cross section ($\sim 20\times 10^{-16}$ cm^2) in this energy region.

II. EXPERIMENT

The experiments were performed using the JILA-ORNL merged electron-ion beam energy loss (MEIBEL) technique, which has several advantages over the crossed-beams fluorescence method that has provided the majority of the cross-section data for electron-impact excitation of positive ions [3,9]. MEIBEL has an increased detection sensitivity, a narrower electron energy distribution, and, essential for the present work on resonances in ion excitation, allows the examination of both dipole and nondipole transitions. Details of the MEIBEL apparatus have been given elsewhere [10] and therefore only a brief summary is included here. Electrons are merged with ions using a trochoidal analyzer and demerged with a similar analyzer after interacting with the ions in a region free of electric fields. The apparatus, schematically depicted in Fig. 1, is immersed in a uniform magnetic field (~ 3 mT) parallel to the ion beam extracted from an electron-cyclotron resonance (ECR) ion source. Electrons from the gun enter a region of crossed **E** and **B** fields, the merger, perform two cyclotron orbits and a drift perpendicular to the two fields so that the electrons exit the merger on trajectories with the same velocities as they entered but shifted perpendicular to the entering axis. The electrons are then collinear with the ions during their passage through the 68.5-mm interaction region before proceeding into the second trochoidal analyzer, the demerger, which deflects the primary electrons through a small angle into a Faraday cup collector while dispersing the inelastically scattered electrons through larger angles onto a position sensitive detector (PSD), consisting of a pair of microchannel plates and a

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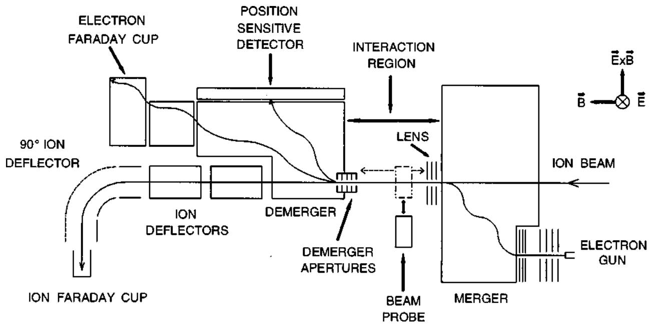

FIG. 1. Schematic view of the merged electron-ion beam energy loss (MEIBEL) apparatus.

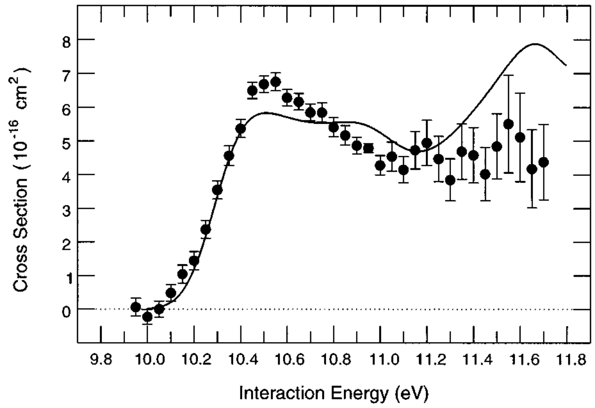

FIG. 2. Cross section vs center-of-mass interaction energy for electrons bombarding Si^{2+} and producing the transition $3s^2\ ^1S \rightarrow 3s3p\ ^1P$. Points represent average experimental values and the bars display the relative uncertainties at 90% confidence level. The solid curve is a convolution of a Gaussian of width 0.24 eV with CCR theory from Ref. [8].

resistive anode. The ions, whose trajectories are not deviated significantly by the demerger fields, are deflected through 90° and collected in another Faraday cup. Electrons elastically scattered through large angles may have similar residual forward velocities to the inelastically scattered electrons and could, in principle, reach the PSD. This is prevented with a series of five apertures placed at the entrance to the demerger. A movable video probe is used to measure the densities of the two beams $[G(x,y,z)$ and $H(x,y,z)]$ at a number of positions along the interaction path in order to compute the overlap of the two beams.

The signal on the PSD is accompanied by large background contributions from electron and ion scattering from residual gas and surfaces, and this requires that both beams are chopped in a phased four-way pattern [10]. The signals, with position and timing information, are accumulated in four histogram memories corresponding to (1) electron background B_e plus ''dark'' background B_d; (2) ion background B_i and B_d; (3) inelastic signal S plus B_e plus B_i plus B_d; and (4) B_d. Before the memory contents can be appropriately added and subtracted to obtain the signal as a function of position on the PSD, it is necessary to correct for the dead time of the detector system. The present configuration [6] of PSD, position computer, and fast first-in-first-out (FIFO) buffers between the position computer and histogram memories leads to a net dead time in the strobe channel of 307.0 ± 0.4 ns and in the rate channel of 60.7 ± 0.1 ns. The counts on the PSD were also corrected position by position for the dead time of the microchannel plates (18 ms per microchannel).

The excitation cross section at an interaction energy in the center of mass system, $E_{\mathrm{c.m.}}$, is determined by

$$\sigma(E_{\mathrm{c.m.}}) = \frac{R}{\varepsilon}\left(\frac{v_e v_i}{v_e - v_i}\right)\frac{qe^2}{I_e I_i}F, \tag{1}$$

where R is the signal count rate from detection of the inelastically scattered electrons, ε the measured PSD detection efficiency, and v_e, v_i, I_e, and I_i are the laboratory velocities and currents of the electrons and ions of charge magnitudes e and qe, respectively. The form factor F is given by

$$F = \frac{\int G(x,y,z)dxdy \int H(x,y,z)dxdy}{\int G(x,y,z)H(x,y,z)dxdydz}. \tag{2}$$

Typical values of the parameters appearing in Eq. (1) for the present study are electron currents of 300 nA, ion currents of 60 nA, and form factors around 3×10^{-3} cm. The signal rates of $\leqslant 2800\ \mathrm{s}^{-1}$ were accompanied by background rates of $B_e \approx 25\,000\ \mathrm{s}^{-1}$, $B_i \approx 5\,000\ \mathrm{s}^{-1}$, and $B_d \approx 50\ \mathrm{s}^{-1}$ for background pressures in the collision chamber of 2×10^{-8} Pa (1.5×10^{-10} torr) and ion energies of 22 and 40 keV. The detection efficiency was measured to be 0.506 ± 0.018.

The data gathering protocol followed that used previously [6] and involved tuning the ion and electron beams to achieve minimum backgrounds while maintaining a reasonable overlap of the beams in front of the demerger apertures but no overlap behind them in order to avoid any elastic scattering beyond the apertures. The beam profiles were then measured and the form factor determined. Data were collected at a particular electron energy until adequate statistical uncertainties were achieved. The electron energy was then adjusted in order to change the interaction energy with careful scaling of the magnetic field and the voltages associated with the electron gun, merger, and demerger to maintain the electron beam profile. Thus, over a range of energies the form factors were not determined other than at the beginning and end of the range as a check on consistency. A number of data runs covering the same energy range were made and averages of these measurements are presented in Figs. 2 and 3.

The measured excitation cross sections for the Si^{2+}:$3s^2\ ^1S \rightarrow 3s3p\ ^1P$ transition were fitted to the convolution of a Gaussian energy distribution of variable width with a step function at 10.28 eV, the spectroscopically determined threshold energy [11]. This procedure gave a full width at half maximum (FWHM) spread in the interaction energy of 0.24 ± 0.02 eV and a necessary shift in the energy scale due to a ''contact potential'' of 2.09 V, which was used to correct all laboratory electron energies. This fitting procedure is the same as that used previously [6], but, in the present case, this dipole transition appears to have a resonance associated with the threshold (see Fig. 2) that may make the use of a step function somewhat suspect. However, the excellent agreement for the energy spread with that determined [6] for Ar^{6+} seems to validate the procedure and was therefore used to determine the width of the Gaussian convoluted with the theoretical results in order to compare with experiment.

Ions from the ECR source are accelerated through a fixed potential, then momentum analyzed so that only particles of fixed $M/q=14$ are in the analyzed beam. Mass spectra indicated that beam contamination due to nitrogen ions was less than 1%. It was expected that a significant fraction of the Si^{2+} ion beam would be in the metastable $3s3p\ ^3P$ state and therefore, in order to determine the fraction, f_m, the ion beam was redirected into the ORNL crossed-beam apparatus [12]. The electron-impact ionization signal below the energy threshold for ionizing ground-state ions, i.e., $27\leqslant E\leqslant 35$ eV, was attributed to the metastable ions and these data resulted in a determination of $f_m=0.301\pm0.014$, in reasonable agreement with a previous result [13] for a similar ECR ion source. Thus, a correction of $(1-f_m)^{-1}=1.431$ was applied to the measured cross sections for excitation from the $3s^2\ ^1S$ ground state.

For electron energies sufficiently above the threshold for an excitation, the scattered electron velocity in the c.m. frame may be such that backscattered electrons (in the c.m. frame) may not move forward in the laboratory frame and thus may not proceed into the demerger and onto the PSD. This limits the energy exceeding the threshold energy for which one can determine the cross sections without corrections for lost signal. In the present case, this is a major limitation as the maximum ion energy possible for a doubly charged ion from the ECR source is approximately 40 keV. For the two ion energies used, 22 and 40 keV, the maximum electron energies without the need for a correction are 0.43 and 0.78 eV above the excitation threshold, respectively. Also, scattered electrons with sufficient velocity in the laboratory frame perpendicular to the beam axis will have large cyclotron radii and may be intercepted by the demerger apertures leading to further lost signal. As detailed previously [6], the data were corrected using a fully three-dimensional trajectory modeling program [14] for the demerger-detector portion of the instrument with the electrons starting from coordinates determined from the beam probe data and their initial trajectories weighted by the theoretical differential cross sections. The angular distribution of the cross sections differed significantly for energies that could be labeled as resonance or nonresonance (background) dominated contributions [8]. Modeling was performed for both types of differential cross sections and, typically, the correction factors differed by less than 10%. The data presented here have correction factors due to backscattering in the range of 1.0–2.0; no data have been included where modeling indicated correction factors greater than 2. This decision restricted the ^3P excitation data to a maximum interaction energy of 7.25 eV for 22-keV ions and 7.56 eV for 40-keV ions with no correction for signal loss necessary (i.e., a correction factor of 1.0) below 6.85 eV for 22-keV ions and below 6.91 eV for 40-keV ions. The equivalent limits in the case of the dipole transition, where only 40-keV ions were used, were a maximum interaction energy of 11.70 eV with no correction needed below 10.65 eV.

A persistent signal below threshold was observed for both the singlet and triplet excitations. In the case of the ^1P data this was determined from the fitting procedure for the energy

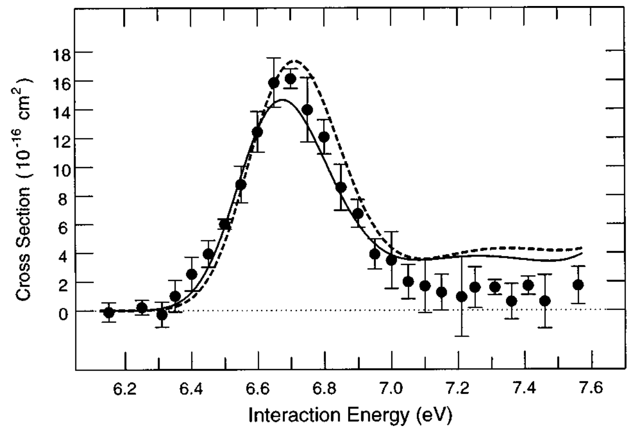

FIG. 3. Cross section vs center-of-mass interaction energy for electrons bombarding Si^{2+} and producing the transition $3s^2\ ^1S\rightarrow 3s3p\ ^3P$. Points and bars are as in Fig. 2. The solid curve is a convolution of a Gaussian of width 0.24 eV with CCR theory from Ref. [8] and the dashed curve is a similar convolution with CCR theory from Ref. [7].

resolution to contribute a constant $(1.316\pm0.036)\times10^{-16}$ cm^2 to the measured cross sections below threshold. Part of the signal is probably due to inelastic scattering producing the $3s3p\ ^3P\rightarrow 3p^2\ ^3P$ transition whose threshold is 9.56 eV. For the measured metastable fraction of 0.301, one would expect [15] a contribution of approximately 1×10^{-16} cm^2 to the measured cross section. The value determined from the fitting procedure has been subtracted from the cross sections displayed in Fig. 2. For the triplet measurements this signal appeared to vary for the separate data runs, making a contribution to the cross sections between 0 and 3.87×10^{-16} cm^2. For this reason, the particular value for this spurious background contribution has been subtracted from each data set before they were combined and presented in Fig. 3.

The relative uncertainties, which have no correlation between data points, are determined by the quadrature sum of uncertainties resulting from counting statistics and uncertainties resulting from the incomplete collection of signal as determined by modeling (20% of the correction). The total relative uncertainties are presented at the 90% confidence level (CL). The combined absolute uncertainty [16] U, also at a 90% CL, includes systematic uncertainties that do not affect the shape of the data. Thus, added in quadrature, there are uncertainties resulting from the metastable content of the ion beam (8%); the spatial delimitation of the signal on the PSD (3%), background subtraction (15%), signal detection efficiency (6%), form factor (15%), and currents (1% each) of the electron and ion beams. The uncertainty due to spurious signals does not include a contribution from the assumption that this background may be subtracted nor that it may vary from one data set to another (in the case of the triplet excitation). Uncertainties in the detector dead times, the particle velocities, and the N^+ contamination of the ion beam were considered negligible compared to the other uncertainties. A coverage factor, $k=1.7$, was used to make systematic uncertainties comparable to 90% CL. Typical values of U are 25.3% for the singlet excitation and 27.7% for the triplet excitation.

III. EXPERIMENTAL RESULTS

A. $3s^2\ {}^1S \rightarrow 3s3p\ {}^1P$

The results for excitation of the dipole-allowed transition [17] are shown in Fig. 2. The solid curve represents the R-matrix close-coupling calculation of Griffin *et al.* [8], convoluted with a Gaussian electron energy distribution of 0.24-eV FWHM. The bars on the points display the relative uncertainty at 90% confidence level. As discussed above, there are additional systematic uncertainties of 23.7%. These data were obtained with a 40-keV ion beam and have been corrected for energies greater than 10.60 eV for backscattering signal loss as outlined above.

The agreement between experiment and theory is mixed. The experimental data give slightly higher cross sections near threshold with the theoretical results larger at higher energies. One may speculate that the resonance responsible for the second bump in the calculated curve at about 10.9 eV may lie at a lower energy, which could improve the agreement between theory and experiment in this lower-energy region. The experimental data also suggest that the higher-lying resonance (near 11.7 eV) may not make as large a contribution to the cross section as predicted and may occur at slightly lower energies. In the light of the larger uncertainties in the higher energy region these suggestions should be considered speculative.

B. $3s^2\ {}^1S \rightarrow 3s3p\ {}^3P$

The experimental cross sections for this spin-forbidden transition [17] are shown in Fig. 3 where they are also compared to two similar close-coupling calculations [7,8]. Both calculations predict very strong resonance structure in the threshold region, which is confirmed by our experiments. The agreement between our results and both calculations is within the relative uncertainties in the threshold region but somewhat poorer above approximately 7.00 eV. But again, it is in this higher-energy region where we suffer through loss of signal and rely on modeling to correct the data. Unfortunately, the higher-lying resonances could not be investigated with the ion energies available from the present ion source.

IV. CONCLUSIONS

The data presented in this paper again demonstrate experimentally the importance of resonances in the electron-impact excitation of positive ions. These data confirm the resonance domination of the cross section for excitation from the ground state to the lowest-lying excited state $(3s3p\ {}^3P)$ of Si^{2+} in the near-threshold energy region as predicted by CCR theoretical methods. The experimental results for the first dipole-allowed excitation of the ground state indicate that resonance locations may have to be more accurately determined to improve the calculated cross sections. A similar conclusion was also reached in our previous work with Kr^{6+} and Ar^{6+} targets, but in those cases it was reached through consideration of nondipole excitations. It is also interesting to note that for the spin-forbidden excitation in Ar^{6+} the agreement between experiment and CCR results was quite poor in the threshold region but excellent for the higher-lying resonances while, in the present case, the converse is true, i.e., we have excellent agreement in the threshold region.

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