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Discrete Deposition of Energy by Electrons in Gases*

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Much previous work on the energy deposition of electrons in gases has centered on the continuous-slowing-down approximation, the key element being the loss function $-(1/n)dE/dx$. Calculations generally reduce to energy integrals involving cross sections and this loss function. The limits of the continuous approximation are now examined by comparing it over various energy intervals with a method which takes into account the discrete nature of the energy lost in each collision. The calculation at each stage considers how an electron at a particular energy will redistribute itself on average at all lower energies, with the distribution depending on cross sections and transition energies. Results of the present work for He and N_2, and comparisons to the continuous approximation, are given.

I. INTRODUCTION

An important aspect of upper atmospheric research involves the question of how an energetic electron incident on a gas populates the various atomic and molecular states it can excite. For example, recent studies of this nature, applied to the calculation of spectral intensities of auroral and dayglow lines, have been carried out by several authors.[1-4] For reasons of its great convenience, the continuous-slowing-down approximation (CSDA) is generally used in these applications whereas the real situation is more in the nature of a random-walk problem. Here the electrons degrade their energy by a series of quantum jumps rather than by the CSDA assumption of continuous energy loss.

The question of how well the CSDA does is, of course, not a new one. Wilson[5] in the precomputer era of physics studied electron and photon initiated showers in lead by Monte Carlo probability wheel methods. Fano[6] and Spencer and Fano[7] in an analysis of range and energy loss of ionizing radiations in matter were concerned with the effects of occasional very large losses due to bremsstrahlung. They discussed an integral equation describing the discrete loss and then combined approximate solutions of it with CSDA to obtain a scheme involving both descriptions.

What is needed for present purposes is a careful examination of CSDA at all energies of interest to atmospheric physics. It is clear that for a sufficiently low-energy electron incident on a gas, the CSDA will predict too small an energy given up to the various states on average. This point may be illustrated convincingly by considering the energy loss of a 25-eV electron in helium. Helium is a rather special case among atmospheric gases in that all the cross sections describing single-electron excitations or ionizations have thresholds bunched together between 19.8 and 24.6 eV. Thus a 25-eV electron will on average lose 22 or 23 eV on its first (and only) collision. On the other hand, the CSDA, which involves an integration over energy from 25 eV down to the lowest threshold at 19.8, predicts a loss of only about 5 eV. The arguments just presented for He do not lead to such obvious conclusions when applied to gases having thresholds widely distributed in energy nor when applied to high energies. Further complications are present when the incident particles have a spectrum of energies.

The present study investigates under what conditions the CSDA is valid with respect to applied problems. The model gases are He and N_2 using the complete sets of semiempirical cross sections given by Jusick *et al.*[8] for He and tabulated by Peterson *et al.*[9] for N_2. Only cross sections for electronic transitions have been included, but, as will be indicated in the results, the inclusion of other cross sections tends to make the continuous approximation more, rather than less, reliable. Hence the results of this work indicate an upper limit to the discrepancies.

II. ENERGY DEGRADATION

A. CSDA

The CSDA, as used in the most recent work of Peterson and Green[10] in calculating the ionization yields of atmospheric gases and of Green *et al.*[3] applied to aurora and airglow spectral intensities, is the basis of comparison in the present study. The population of each state in He and N_2 is computed after complete energy degradation of an incident primary electron and of all the resulting secondaries. The number $J_j{}^0(E_p)$, defined as the population of state j after degradation of the primary alone from energy E_p, satisfies the equation

$$J_j{}^0(E_p)=\int_{W_j}^{E_p}\frac{\sigma_j(E)}{L(E)}\,dE\quad, \tag{1}$$

where W_j is the threshold of the state j and $L(E)$ is the loss function $-(1/n)dE/dx$. A similar expression may be written for ionization states. The secondary electron spectrum resulting from ionization of state i is given by

$$n_i(E_p,E_s)=\int_{2E_s+I_i}^{E_p}\frac{S_i(E,E_s)}{L(E)}\,dE\quad, \tag{2}$$

where E_s is the secondary electron energy and I_i is the ionization potential. Having obtained the population $J_j{}^0(E_p)$ arising from primaries alone, the total population of state j after secondaries are also degraded comes from the integral equation

$$J_j(E_p)=J_j{}^0(E_p)+\sum_i\int_0^{(E_p-I_i)/2}J_j(E_s)n_i(E_p,E_s)dE_s\quad. \tag{3}$$

The above equations are very convenient in applied problems. Using power series functional forms for the various cross sections as well as for the inverse loss function in the manner of the above references, Eqs. (1) and (2) may be integrated directly. Equation (3) is easily done numerically.

B. Discrete Loss

In carrying out the degradation by means of discrete steps one must, in some way, follow typical electrons as they perform successive collisions. The usual problem begins with a single electron having energy E_p, and ends when, after a series of collisions, the electron and all its secondaries have energies less than the lowest threshold of interest.

To accomplish the energy degradation in a convenient way, the energy scale 0 to E_p is divided into a reasonable number of equally spaced points which define the centers of what are referred to as bins. One electron is placed in the bin labeled p, and zero electrons in all other $p-1$ bins. This one electron, as a result of the first collision, will redistribute itself fractionally in an average sense in the lower bins, as controlled by the various cross sections. The topmost bin having been emptied, one can now proceed to the next bin, and redistribute any electrons or fractional parts of an electron which had been dumped there. This process continues until all bins of interest are empty.

All events leading to an energy loss less than a bin width are ignored for simplicity. Rotational and vibrational excitations are not considered, nor are losses due to elastic scattering, and, partly because of this, bin widths of 0.2–1.0 eV are adequate. If any neglected cross sections are large enough so that, on average, several low-loss events take place before a high-loss event occurs, then the accumulative effects can be significant. These effects are not in the spirit of this somewhat simplified study, however.

The probability of exciting the state j, causing the electron in bin p to jump to another bin, is proportional to the cross section $\sigma_j(E_p)$. Therefore, if we have the total effective cross section $\sigma_{\text{eff}}(E_p)$ for events contributing to a jump in bins, the probability for changing bins via the jth channel is

$$P_j(E_p)=\sigma_j(E_p)/\sigma_{\text{eff}}(E_p)\quad. \tag{4}$$

Of course, once the particular channel is defined, the particular bin the electron goes to is determined by the transition energy W_j. It is important to recognize that $\sigma_{\text{eff}}(E_p)$ is not the total cross section but is rather the effective "bin jump" cross section.

In considering the events leading to an ionization, the differential cross section $d\sigma_i(E_p,E_s)/dE_s$ must be used. The expression analogous to Eq. (4) which will represent the probability for an electron in bin p exciting the ith state of ionization, ejecting a secondary of energy between E_s and $E_s+\Delta E_s$, and losing energy I_i+E_s, is

$$P_i(E_p,E_s)=\Delta\sigma_i(E_p,E_s)/\sigma_{\text{eff}}(E_p)\quad, \tag{5}$$

where

$$\Delta\sigma_i(E_p,E_s)=\frac{d\sigma_i(E_p,E_s)}{dE_s}\Delta E_s\quad. \tag{6}$$

Of the two outgoing electrons, the one with lower energy is considered to be the secondary, and the other one the primary. This implies that the upper energy limit to the secondaries from ionization state i is $\frac{1}{2}(E_p - I_i)$. The total cross section for an ionization leading to state i is the sum over all allowed values E_s of $\Delta\sigma_i(E_p, E_s)$ plus any contributions from autoionization via quasibound compound states above the ionization threshold I_i. Autoionization secondaries will produce spikes in the low-energy secondary electron spectra and will contribute to low-lying states. However, we have ignored this effect, because He and N_2 do not have low-lying electronic states.

A formidable array of tabulated information would be needed to do the problem completely numerically. For this reason it is very convenient to use functionally parametrized cross sections of the type suggested by Green.[11] In their most recent forms, the cross sections for electronic excitations are written as

$$\sigma_j(E) = (q_0 f_0 c_0 / W_j^2)(W_j/E)^{\Omega} \sum_s a_s (W_j/E)^{\Gamma_s} \quad , \qquad (7)$$

where q_0 is the constant 6.514×10^{-14} $\mathrm{cm^2\,eV^2}$, $f_0 c_0$ is a strength parameter, W_j is the transition energy, and where Ω, a_s, and Γ_s are shape parameters. The differential ionization cross section $d\sigma(E, E_s)/dE_s$ [or what is the same, $d\sigma(E, W)/dW$, where the continuous energy loss W is defined by $W = I_i + E_s$] is

$$\frac{d\sigma(E, W)}{dW} = \frac{q_0 A_0}{W^2}\left(\frac{I_i}{W}\right)^{p}\left(\frac{W}{E}\right)^{\Omega}\sum_s a_s\left(\frac{W}{E}\right)^{\Gamma_s} \quad . \qquad (8)$$

In the above parametrization, p controls the W dependence for fixed E, whereas Ω and the sets (a_s, Γ_s) control the E dependence for fixed W. The functions (7) and (8) do a rather remarkable job of fitting the smoothed cross sections.

In the method of computation used, it is necessary to carry the calculations through a complete depletion of all bins above the thresholds of the states under examination. The method is clearly unphysical when stopped before completion, unlike a Monte Carlo type calculation where a large number of single electrons are followed down to any desired energy from an initial value. This unphysical characteristic of the method, however, is not a real problem. If, for example, one wanted to know the average effects of an electron having initial energy E_p degrading to a final energy E_f, a complete calculation from E_p to threshold can be done, followed by one from E_f to threshold, and the results can then be subtracted. This technique is of special value when comparing the results of the present method to those of the CSDA, where integrations over energy from E_p to E_f can be done rather easily.

III. RESULTS

In the present application, the program for discrete degradation is first run by allowing only the primary electron to degrade from various initial energies. The secondary electrons are accumulated from this calculation to produce a spectrum for each initial energy. The same program is then rerun, this time allowing the secondaries to degrade as well. These two runs give the three quantities $J^0(E_p)$, $J(E_p)$, and $n(E_p, E_s)$, with which the CSDA can be compared. Starting from the identical cross sections, the CSDA calculation is performed by first computing the loss function $L(E)$ directly from the cross sections, and then using Eqs. (1)–(3) for the above quantities.

It is of practical interest to note that a bin width as large as 1 eV is sufficient for most purposes. It is only for sharply peaked forbidden transitions that a smaller bin width of 0.2 eV is sometimes needed. Even with 1-eV bins a running check during and after computation shows that the total energy of the system remains within 1% of the original energy of the primary electron. Furthermore, because in the degradation from successive initial values many of the computer operations are identical, it is possible to do a large number of starting energies with little increase in computer time over what is spent in degrading from a single energy. A typical run for He using 1-eV bins and $E_p = 500$ eV takes about 3 min on an IBM 360-50. The time increases roughly as the square of the number of bins, and linearly as the number of ionization states.

A. He

Any process leading to double excitation or double ionization is neglected. All single-electron excitation cross sections in He are included by fitting functions of the form of Eq. (8) to the semiempirical cross sections of Jusick *et al.*,[8] with the higher rydberg members $n = 4$ to ∞ summed in each case to an effective single cross section. The differential ionization cross section is fitted with a function of the form of Eq. (9), and is parametrized in the same manner by Peterson and Green,[10] who determined the best set of parameters to provide consistency between the cross sections, the loss function, and the energy per ion pair. Computing the discrete degradation as described earlier, the points in Figs. 1–3 are generated. When dealing with ionization the results are translated from population number $J(E)$ to energy per ion pair, defined by $E/J(E)$, as is customarily done. The identical cross sections, used in a CSDA calculation, yield the solid and dashed curves on the same figures.

Several important features are immediately apparent. First, the discrete calculation pre-

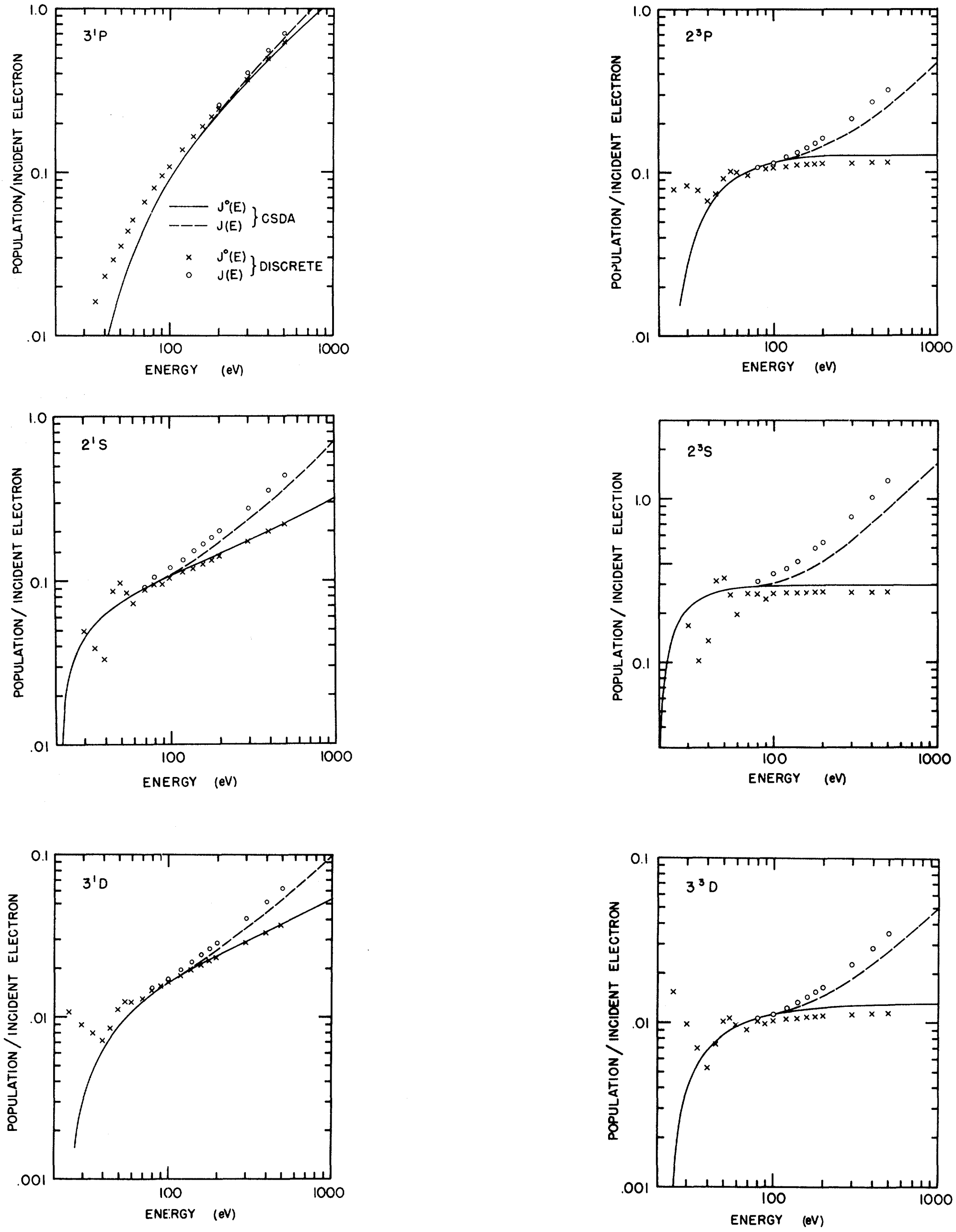

FIG. 1. Average populations of various states in He as a function of incident electron energy, according to the CSDA and discrete methods.

dicts rapid fluctuations in population at low energies, but these fluctuations fade as energy increases. The secondary spectra predicted by the two methods approach each other for high initial primary energies. However, there is a tendency for the CSDA to underestimate the number of high-energy secondaries, the effect being more pronounced for low primary energies. This means that the contributions from secondaries are a lower percentage of the total populations in the CSDA than is shown in the discrete study. Figure 1 also points out the differences between allowed- and forbidden-state populations. Allowed states are in general very well represented by the CSDA compared to the discrete calculation, and, in fact, the two results tend to merge at high energies. Forbidden states, on the other hand, are only moderately well represented. The basic differences between allowed and forbidden states come from the fact that, whereas allowed states

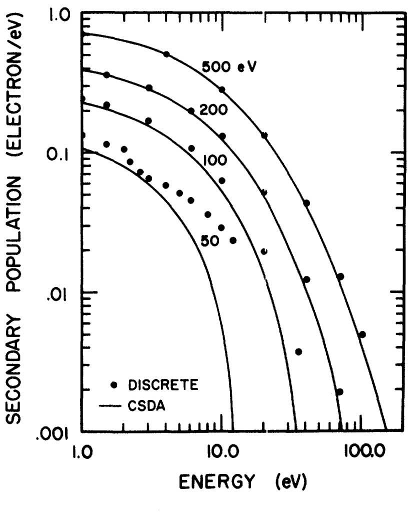

FIG. 2. Average spectra, according to the CSDA and discrete methods, of secondary electrons in He resulting from incident electrons at various starting energies.

are populated mostly from primaries, forbidden states are populated mostly by secondaries or low-energy primaries. The energy region of importance to forbidden states is the region below 100 eV, where the CSDA begins to break down.

The eV per ion pair calculation shows that CSDA provides a reasonable estimate at high energy but, as expected, breaks down as the primary energy approaches threshold. As seen in Fig. 2 the region 30–40 eV shows the fluctuations mentioned earlier, which CSDA cannot describe.

B. N_2

Similar comments apply to N_2 as to He, but there are several important differences. Since N_2 has many ionization continua the cost of a discrete calculation is much higher than for He, which has only one single-electron ionization state. For that reason it is especially desirable that the CSDA works well. The thresholds of the various states of N_2 are spread out in energy, a different situation than exists in He. The spreading out of thresholds has the effect of reducing the fluctuations and improving the over-all performance of the CSDA. Figures 4 and 5 illustrate some representative results for N_2. Although the population due to primaries alone for forbidden states still shows wide discrepancies, the total populations from the two methods are in good agreement at high energy. Allowed states and also ionization states, which are not shown, indicate good agreement . It is expected that the consideration of molecular vibrations and rotations will further improve the agreement since the thresholds are made even more diffusely spread out.

IV. CONCLUSIONS

The results are, on the whole, rather encouraging, since it is the low-energy region that is almost entirely responsible for the breakdown of the CSDA. Even with this low-energy breakdown, enough regularities exist in the discrepancies between the two methods to say that, at high energies, the CSDA usually underestimates forbidden-state populations by from 0–50%, whereas it only slightly underestimates allowed states.

The type of application dictates whether or not the detailed discrete degradation approach is needed. In upper atmospheric research it is presently unrealistic to attempt to reproduce experimental results to better than factors of about 2. The reasons come from the complexity of the phenomena in which only approximately known cross sections interact in a medium that shows large variations in such variables as density and precipitating energy. Thus, until these uncertainties can be reduced, the CSDA remains acceptable. For more precise measurements, however, like ion yields at low energy, the CSDA is obviously poor, although at high energy the situation is again reasonable.

Additional support for CSDA for most applications in atmospheric work comes when one imagines the effects in a discrete calculation of the incident particles that have a large spread in energy. The fluctuations shown in the figures would be effectively averaged out. One can further imagine the limit as many gases are mixed together. Here the tendencies exhibited by N_2 in comparison to He should be even more enhanced. Very low-lying states such as exist in O and O_2 have not been treated here, however, and are candidates for special study.

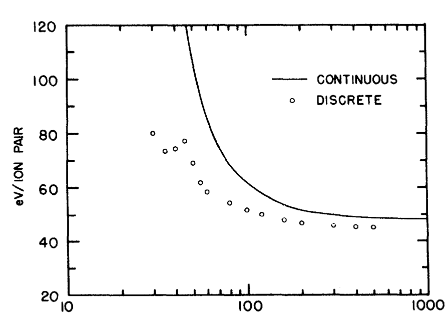

FIG. 3. Energy per ion pair for He as a function of incident electron energy, according to the CSDA and discrete methods.

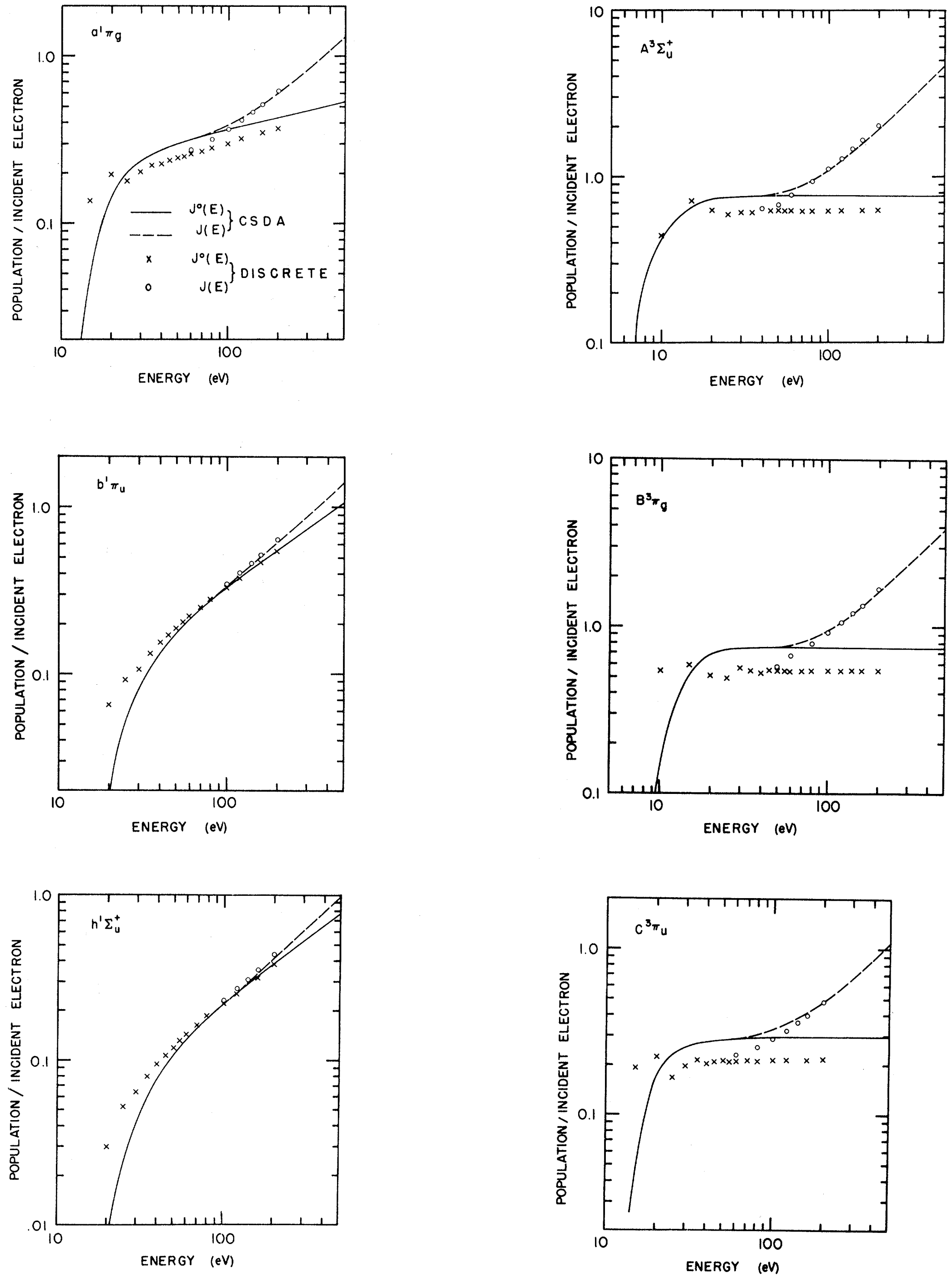

FIG. 4. Average populations of various states in N_2 as a function of incident electron energy, according to the CSDA and discrete methods.

For the future, in view of the results of the present work, it is reasonable to assume that techniques can be developed in which the CSDA is used in conjunction with low-energy corrections to provide good results at all energies. One obvious improvement is to carry the CSDA calculation from keV energies down to 100–200 eV, and then feed the results into a discrete contin-

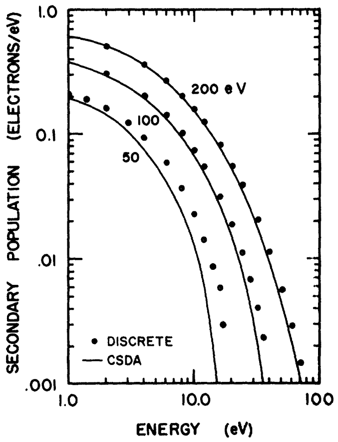

FIG. 5. Average spectra, according to the CSDA and discrete methods, of secondary electrons in N_2 resulting from incident electrons at various starting energies.

uation down to threshold. Phenomenological modifications of CSDA parameters based on observed regularities in the discrepancies may also be possible.

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Threshold Electron-Impact Excitation of the 5s Electron in Xenon[†]

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The threshold electron-impact excitation of the 5s electron in xenon has been studied, using electron scavenging by sulfur hexafluoride. Optically forbidden states are preferentially excited.

Samson[1,2] has studied optical excitation in xenon to discrete states in the continuum above the first ionization potential. Transitions of the type $5s^25p^6 \rightarrow 5s5p^6np$ are observed. In a separate study in the same energy range, Madden and Codling[3] have reported the discovery of autoionizing atomic energy levels of xenon, using electron synchotron radiation. Because of configuration interac-