Ionization Produced by Atomic Collisions at kev Energies. II*†

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The electron evaporation model, presented in a previous paper, of the collision-ionization process that occurs when atoms collide at high energies is extended and improved. In addition, an alternate model of the process is considered. This second model treats the collision-ionization process as being due to direct knock-outs of the electrons by violent electron-electron collisions. It is found that this model cannot be made to account for the data, thereby lending additional support to the assumptions inherent in the evaporation model.

1. INTRODUCTION AND SUMMARY OF RESULTS

IN a previous paper,[1] hereafter referred to as I, a phenomenological theory was developed to account for the ionization produced by violent atomic collisions. The purpose of the present work is to extend and improve the theory as there presented.

In essence, the model of the collision-ionization process presented in I consists of two separate parts: First, as the two electron clouds sweep through each other during the collision, a relatively small amount of the kinetic energy of translation of the atoms is transferred to their internal degrees of freedom by a friction-like mechanism. Second, upon separation, the "heated atoms" get rid of this excess energy partly by photon emission and partly by electron evaporation. Insofar as the electron evaporation part of the theory is concerned, the energy transferred to the internal degrees of freedom is statistically distributed among the eight outer electrons.

This distribution was effected, in I, by dividing the energy scale into cells of equal width ϵ, and then calculating the ionization probabilities algebraically. To make the problem tractable, the size ϵ of the energy cell was there taken to be one quarter of the ionization energy (assumed to be the same for all ionization states).

The statistics have since been improved by going to the limit $\epsilon \rightarrow 0$.[2] The resulting $\bar{P}_n(E_T)$ curves are, except for a lateral shift to slightly higher values of E_T, almost superimposable on the original curves (Fig. 3 of I) obtained with ϵ equal to one quarter of the ionization energy. The discrepancies are less than 5% of the peak heights, when the original curves are shifted to higher values of E_T by an amount equal to the ionization energy. Inasmuch as the transformation of abscissa from E_T to θ involves an empirically adjusted constant, the limiting $\bar{P}_n$ curves do not yield significantly different agreement of the over-all theory with experiment to warrent redrawing Figs. 11 and 12 of I.

A more important improvement of the theory deals with the energy E_T transferred to the internal degrees of freedom during the atomic collision. In I, this energy was assumed to be a single valued function of the collision parameters as shown by Eq. (9) of I. Thus, no provision was there made to allow for a statistical distribution in E_T. This implicitly assumes that so many electron-electron collisions are involved in the energy transfer process that the statistical distribution in this quantity can be neglected. (Although a statistical distribution *in* the values of E_T was not considered in I, the statistical distribution *of* the energy E_T among the outer electrons was considered in that paper.)

However, the experimental results of Afrosimov and Federenko[3] indicate that there may be a substantial spread in the distribution in E_T for a given set of collision parameters. Therefore, in Sec. 2, the theory of I is generalized to allow for a statistical distribution in this quantity. It is found that the effect of this generalization does not affect the agreement with experiment of the uniform ionization potential evaporation theory.

Finally, in Sec. 3, an alternative phenomenological theory of the collision-ionization process is considered, for the sake of completeness. This second model, which will be referred to as the "stripping" model (in distinction to the "evaporation" model considered heretofore), regards the ionization as produced by violent electron-electron collisions in which the colliding electrons are knocked directly out of their respective atoms. It is found that this "stripping" model cannot be made to account for the experimental data.

2. THE DISTRIBUTION IN E_T

The theory presented in I tacitly assumed that the number of electron-electron collisions involved in producing E_T was sufficiently large so that there was no appreciable spread in the distribution of this quantity

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TABLE I. Comparison of theory and experiment.

Point	Exp.	Unif. evap.	Δ	Av. unif. evap.	Δ	Stag. evap.	Δ	Av. stag. evap.	Δ	Knockouts	Δ
$\tilde{P}_1\times\tilde{P}_2$	0.42	0.42	0.00	0.36	0.06	0.52	0.10	0.48	0.06	0.29	0.13
$\tilde{P}_0\times\tilde{P}_3$	0.08	0.09	0.01	0.14	0.06	0.00	0.08	0.02	0.06	0.15	0.07
$\tilde{P}_2$	0.47	0.46	0.01	0.39	0.08	0.75	0.27	0.67	0.20	0.29	0.18
$\tilde{P}_0\times\tilde{P}_4$	0.06	0.02	0.04	0.06	0.00	0.00	0.06	0.00	0.06	0.10	0.04
$\tilde{P}_1\times\tilde{P}_3$	0.23	0.25	0.02	0.24	0.01	0.13	0.10	0.17	0.06	0.22	0.01
$\tilde{P}_1\times\tilde{P}_4$	0.14	0.11	0.03	0.14	0.00	0.02	0.12	0.04	0.10	0.16	0.02
$\tilde{P}_2\times\tilde{P}_3$	0.34	0.39	0.05	0.33	0.01	0.48	0.14	0.46	0.12	0.24	0.10
$\tilde{P}_3$	0.37	0.42	0.05	0.37	0.00	0.67	0.30	0.62	0.25	0.24	0.13
$\tilde{P}_0\times\tilde{P}_5$	0.03	0.00	0.03	0.02	0.01	0.00	0.03	0.00	0.03	0.07	0.04
$\tilde{P}_2\times\tilde{P}_4$	0.24	0.25	0.01	0.24	0.00	0.18	0.06	0.20	0.04	0.19	0.05
$\tilde{P}_1\times\tilde{P}_5$	0.06	0.04	0.02	0.07	0.01	0.00	0.06	0.00	0.06	0.12	0.06
$\tilde{P}_3\times\tilde{P}_4$	0.33	0.35	0.02	0.32	0.01	0.46	0.13	0.45	0.12	0.20	0.13
$\tilde{P}_2\times\tilde{P}_5$	0.14	0.13	0.01	0.15	0.01	0.04	0.10	0.05	0.09	0.15	0.01
$\tilde{P}_0\times\tilde{P}_6$	0.01	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.01	0.05	0.04
$\tilde{P}_4$	0.37	0.37	0.00	0.36	0.01	0.57	0.20	0.54	0.17	0.20	0.17
$\tilde{P}_1\times\tilde{P}_6$	0.02	0.01	0.01	0.03	0.01	0.00	0.02	0.00	0.02	0.09	0.07
$\tilde{P}_3\times\tilde{P}_5$	0.24	0.24	0.00	0.24	0.00	0.24	0.00	0.24	0.00	0.17	0.05
$\tilde{P}_2\times\tilde{P}_6$	0.06	0.07	0.01	0.08	0.02	0.00	0.06	0.00	0.06	0.12	0.05
$\tilde{P}_4\times\tilde{P}_5$	0.32	0.32	0.00	0.32	0.00	0.39	0.07	0.39	0.07	0.18	0.14
$\tilde{P}_3\times\tilde{P}_6$	0.14	0.14	0.00	0.16	0.02	0.10	0.04	0.12	0.02	0.15	0.01
$\tilde{P}_1\times\tilde{P}_7$	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.07	0.07
Mean Error			0.016		0.016		0.093		0.076		0.075

for given collision parameters. As was pointed out in the Introduction, however, there is experimental evidence that this is not so. Therefore, the effect on the conclusions of I caused by a distribution in E_T will be considered in this section.

Equation (9) of I must now be regarded as a relation between average values:

$$\bar{E}_T=\bar{\nu}\bar{e}_T, \quad (1)$$

where $\bar{\nu}$ is the average number of electron-electron collisions and $\bar{e}_T$ is the average energy transferred per collision. The distribution in E_T will then be assumed to be a Gaussian distribution about $\bar{E}_T$ as mean, with a standard deviation Δ proportional to $\bar{E}_T^{\frac{1}{2}}$.

$$\Delta=\alpha\bar{E}_T^{\frac{1}{2}},$$

$$G(E_T,\bar{E}_T)=(2\pi\Delta^2)^{-\frac{1}{2}}\exp[-(E_T-\bar{E}_T)^2/2\Delta^2], \quad (2)$$

where $G(E_T,\bar{E}_T)dE_T$ is the probability that, in the overall atomic collision, the energy transferred to the internal degrees of freedom lies between E_T and E_T+dE_T when the expected value is given by $\bar{E}_T$.

In this connection, it may be worthwhile to remark that the distribution in ν is expected to be the well-known Poisson distribution:

$$F(\nu)=\bar{\nu}^{\nu}\exp(-\bar{\nu})/\nu!, \quad (3)$$

which, for sufficiently large values of $\bar{\nu}$, reduces to the Gaussian distribution with standard deviation equal to $\bar{\nu}^{\frac{1}{2}}$. A discussion of this assumption is given in Sec. 3. However, the distribution in e_T cannot be obtained at the present stage of the theory, since this quantity has been only vagely defined in terms of an empirically adjusted constant. To attempt greater precision in the definition and calculation of this quantity would be meaningless at this time, in view of the scantiness of direct experimental measurements of E_T against which this part of the theory could be checked. Consequently, all that is being attempted in this paper is a qualitative study of the effect on the evaporation part of the theory of I caused by a reasonable distribution in E_T. The assumption made in Eq. (2) would be valid if the distribution in E_T were predominantly due to the distribution in ν. It is not expected that the distribution in e_T will basically change the overall distribution in E_T.

With a distribution in E_T, the ionization probabilities $\mathcal{P}_n$, at such collision parameters that the expected energy transferred is $\bar{E}_T$, are given by:

$$P_n(\bar{E}_T)=\int_0^\infty G(E_T,\bar{E}_T)\tilde{P}_n(E_T)dE_T. \quad (4)$$

The above averaging process was performed for both the uniform and staggered ionization potential results of I with α set equal to 2. Mathematically, this corresponds to the following: (a) no distribution in e_T, which is taken to be 4 ev; and (b) an ionization potential of 16 ev in the uniform ionization case, and a first ionization potential of 16 ev in the staggered ionization potential case.

The effect of the distribution in E_T is to make the agreement of the uniform ionization potential results become slightly poorer for small values of E_T and

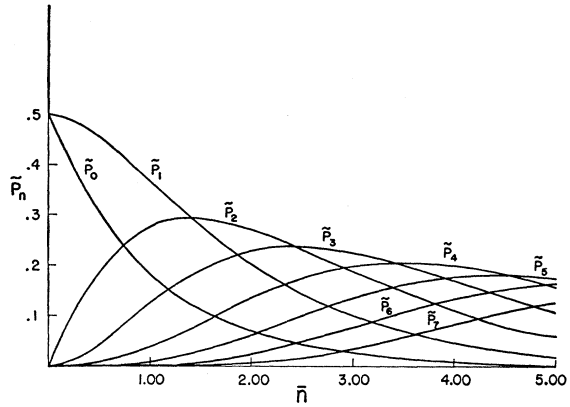

FIG. 1. The ionization probabilities $\tilde{P}_n$, given by Eqs. (5), that follow from the direct knockout, or stripping, model are plotted as functions of $\bar{n}$.

slightly better for large values of E_T, with no net change in the overall agreement. The results of the staggered ionization potential theory are brought more closely in line with the experimental results, but they are still too poor to be acceptable. All these conclusions are quantitatively shown in Table I.

From an examination of the trends, it appears that a *slightly* staggered ionization potential in conjunction with a distribution in E_T about as large as the one considered above would also yield agreement with experiment. However, it is not worthwhile to pursue this point until more complete experimental data concerning E_T is obtained.

3. THE "STRIPPING" MODEL

The theory presented in I is an evaporation theory. It insists that a certain amount of internal energy E_T, generated by the collision, is thoroughly distributed among the outer electrons before ionization occurs. It is by no means clear *a priori* that this must be so. An alternative approach would be to assume that there is little time for an exchange of energy between the electrons of a given atom before ionization takes place. Such an assumption would require that those electrons soundly struck during the over-all atomic collision would be directly knocked out of the parent atom. This idea is implied in the terminology currently being used to describe the collision-ionization cross-sections. They are popularly called the "stripping" cross sections.

To test the validity of such a model of the collision-ionization process, the following assumptions are made: (1) When two electrons, one from either atom, make a particularly violent collision, each will be knocked out of the respective parent atom. Electron-nucleus collisions are assumed not to be a factor in the ionization process. (2) The single initial electron deficiency, present in singly ionized atom-neutral atom collisions, can affix itself with equal probability to either projectile or target, if they are similar.

Using the Poisson distribution [Eq. (3)], where now n, instead of ν, denotes the number of electron-electron collisions, the probability $\tilde{P}_n$ that the observed atom is n-fold ionized is given by:

$$\tilde{P}_0(\bar{n})=\tfrac{1}{2}\exp(-\bar{n}),$$
$$\tilde{P}_n(\bar{n})=\tfrac{1}{2}[\bar{n}^n\exp(-\bar{n})/n!]+\tfrac{1}{2}[\bar{n}^{n-1}\exp(-\bar{n})/(n-1)!]. \quad (5)$$

The first term represents the probability that the observed atom was not the deficient one and had n electrons knocked out, while the second term gives the probability that the observed atom was the deficient one and had $n-1$ electrons knocked out. In either case, the same number of electron-electron collisions occurred, so that $\bar{n}$ is the same for both terms.

Strictly speaking, the Poisson distribution is mathematically valid for randomly timed events in which, on the average, z events occur per unit time. It gives the probabilities that various numbers of events n will occur in a given time interval T, which is related to $\bar{n}$ by

$$\bar{n}=zT. \quad (6)$$

If the time axis were broken up into a great many intervals all of the same duration T, then $\bar{n}$ would be the average number of collisions occurring per interval T.

The use of the Poisson distribution to represent the distribution in the number of electron-electron collisions thus involves a physical assumption of sorts. It is motivated by the reasoning that if, for many identical atomic collisions (i.e., each with the same collision parameters and, therefore, the same collision duration T), the average number of electron-electron collisions that occur per atomic collision is $\bar{n}$, then the probability that n electron-electron collisions will occur in one over-all atomic collision (i.e., in the time T) is given by the Poisson distribution.

The probabilities $\tilde{P}_n$ given by Eq. (5) are plotted in Fig. 1, as functions of $\bar{n}$, which, in turn, is a function of the collision parameters. Thus $\bar{n}$ is the analogue of $\bar{E}_T$ in the evaporation theory. It is not necessary to carry out the last step, however, to see that agreement with the experimental data cannot be achieved. As can be seen in Table I, the peak heights are too low and the heights of the intersections of the various curves are also in very poor agreement with the data. Even more than this, the order of occurrence of the various intersections is also in poor agreement with the experimental data.

Thus, it appears that the direct knock-out, or stripping, model cannot account for the data, thereby lending additional support to the assumptions inherent to the evaporation model.

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