J. Phys. B: Atom. Molec. Phys., Vol. 11, No. 14, 1978. Printed in Great Britain

Threshold behaviour of L x-ray excitation in Xe–Ag collisions†

H O Lutz‡‖, W R McMurray‡, R Pretorius‡, T Morović§, B Fricke§, W D Sepp§ and I J van Heerden‡

‡ Southern Universities Nuclear Institute, Faure, Cape Province, South Africa

§ Gesamthochschule Kassel, D-3500 Kassel, West Germany

Received 16 January 1978, in final form 22 March 1978

Abstract. In the collision system Xe–Ag, the thresholds for excitation of quasimolecular L radiation and characteristic Ag L radiation have been found to lie at about 5 MeV and 1 MeV, respectively. These results are discussed on the basis of *ab initio* calculations of the screened interaction potential and the electron-correlation diagram.

Relativistic Dirac–Slater molecular calculations have been shown to give a good account of the spectral shape of x-radiation excited in collisions between very heavy particles (Fricke *et al* 1976, Lutz *et al* 1976, Morović *et al* 1977). It has been suggested that observation of the threshold behaviour of the excited radiation should provide a check on the details of the theoretical correlation diagrams, e.g., the location of individual level crossings (cf Lutz *et al* (1976) for the Xe–Au system).

In this paper we report on an experimental investigation of the Xe–Ag collision system at and below 9 MeV ion energy, the molecular correlation diagram of which has been calculated by Morović *et al* (1977). A collimated beam of Xe^+ ions from the SUNI 6 MV van de Graaff accelerator (energy calibrated using an NMR probe in the 90° deflection magnet) was directed onto thin Ag targets ($\sim 50\ \mu g\,cm^{-2}$) evaporated on Mylar and Kapton backings, inclined 45° to the incident beam direction; above 4 MeV, Xe^{2+} ions were used. The x-ray emission was detected either through a 28 μm Al absorber (to enhance the continuum part of the spectrum at about 9 keV) or without an Al absorber (to secure information on the low-energy part of the spectrum) in a 28 mm^2 Si(Li) detector placed perpendicular to the ion-beam axis opposite the target.

Figure 1 shows x-ray spectra for different incident ion energies, using the 28 μm Al absorber. The dominant features are the Xe L radiation at about 4 keV x-ray energy, and Ag L radiation at about 3 keV x-ray energy. The broad structure between 7 and 10 keV has been associated with the quasimolecular (MO) L radiation (Morović *et al* 1977); its threshold lies at about 5 MeV ion energy.

To obtain a realistic description of the threshold behaviour, the wavefunction at the active crossings as well as the collision dynamics, including a realistic interaction potential, should be taken into account.

† Supported by the SA Council for Scientific and Industrial Research, and by GSI Darmstadt.

‖ Permanent address: Fakultät für Physik, Universität Bielefeld, D-4800 Bielefeld 1, West Germany.

0022-3700/78/0014-2527 $01.00

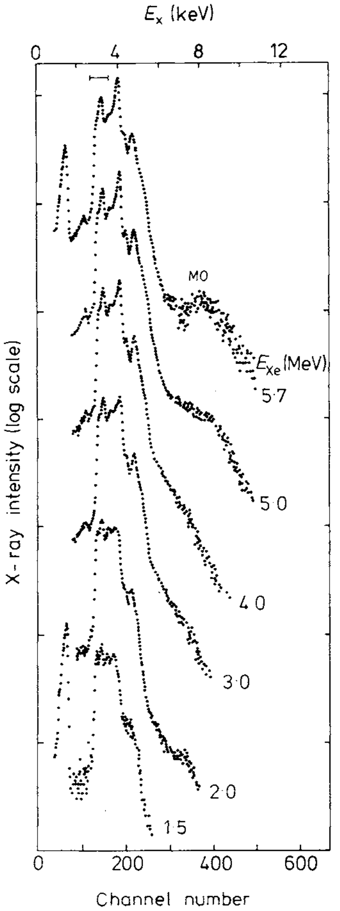

Figure 1. Energy spectra of x-rays excited in Xe–Ag collisions for different laboratory ion energies (Al absorber 28 μm).

The latter has been calculated *ab initio* in a Dirac–Fock–Slater (DFS) treatment of the system Xe^{22+}–Ag^{19+} by computing the difference of the statistical total energies between the isolated atoms and the quasimolecule (cf Baerends *et al* 1973) and adding the nuclear Coulomb potential as a function of the internuclear distance R. The uncertainty ΔV in the interaction potential is determined by the accuracy ΔV_e with which the statistical total energy V_e is calculated; $\Delta V_e/V_e$ is about $\pm 5\%$, resulting in $\Delta V/V \simeq \pm 2\%$ at $R = 0{\cdot}04$ au, and $\Delta V/V \simeq \pm 12\%$ at $R = 0{\cdot}2$ au. The differences between the DFS potential and a pure Coulomb potential V_c are significant; on the other hand, within the range and precision of the calculation it is identical to the screened Bohr potential $V_B = V_c \exp(-R/a)$, with $a = (Z_1^{2/3} + Z_2^{2/3})^{-1/2}$.

A rigorous treatment of the MO L x-ray excitation at threshold, including the proper wavefunctions, has not yet been performed. A rough estimate of the internuclear separation R at which the level crossing occurs may nevertheless be obtained. In a head-on collision at 5 MeV ion energy, the collision partners just penetrate to $R = 0{\cdot}027$ au. According to the correlation diagram (Morović *et al* 1977), this is where the level crossings responsible for excitation of MO L radiation are located.

At lower energies, the collision partners always remain at larger R, and excitation of MO L radiation is suppressed.

The emission of the characteristic Ag L x-rays has been studied by omitting the 28 μm Al absorber in front of the Si(Li) detector. The Ag L radiation yield was obtained by integrating the corresponding spectral peak between 2·65 and 3·75 keV x-ray energy; the energy window is indicated in figure 1. In the ion energy range investigated, the Ag L intensity was about ten times as high as the Xe L intensity. Absolute cross sections were calculated in the usual manner by normalising to the integrated ion-beam charge, and correcting for x-ray detector sensitivity and solid angle. The results are displayed in figure 2 as a function of laboratory ion energy E. The Ag L-excitation curve exhibits a threshold at about 1 MeV. The data points at energies above 4 MeV show a relatively large scatter because the available current of Xe^{2+} ions was very small ($\lesssim 0{\cdot}2$ nA) making current integration somewhat difficult. Due mainly to the uncertainty in the target thickness, the absolute cross sections are uncertain by as much as 50%; the relative uncertainty of the data points is smaller and is indicated in figure 2.

It follows from the correlation diagram calculated by Morović *et al* (1977) that crossings at $R = 0{\cdot}092$ au and $R = 0{\cdot}146$ au contribute to the Ag L x-ray production (note a typing error in Morović *et al* 1977: the second crossing occurs at 0·146 au, not at 0·16 au). From a rough estimate, as performed above for MO L excitation, corresponding thresholds of about 1 MeV and 0·5 MeV ion energy, respectively, are obtained. The threshold at about 0·5 MeV caused by the crossing at 0·146 au is outside the ion energy range studied here. From the correlation diagram we note, however,

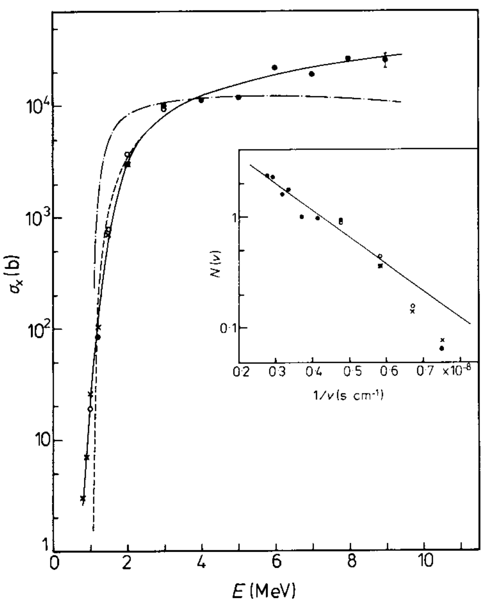

Figure 2. Total cross section for excitation of Ag L radiation in Xe–Ag collisions as a function of laboratory ion energy E (different symbols indicate different sets of experiments). The full curve serves to guide the eye. Chain and broken curves are explained in the text. The relative experimental uncertainty is given by the error bar. The absolute scale is uncertain by as much as 50%. Insert: number $N(v)$ of vacancies feeding the crossing at $R = 0{\cdot}092$ au plotted against reciprocal ion velocity, v^{-1}.

that this crossing is fed by low-lying σ levels which correlate to the Xe 3s and $3p_{1/2}$ subshells. These levels are expected to have a smaller vacancy-occupation probability than those feeding the crossing at 0·092 au; the latter belong to a set of orbitals correlating to the more weakly bound Ag M shell. Thus, at 1 MeV ion energy only a small influence of the crossing at 0·146 au is expected. We therefore attempted a description of the threshold behaviour at 1 MeV neglecting any contribution of this outer crossing. According to the correlation diagram, the excitation occurs via radial coupling at a well defined internuclear separation; this is corroborated by the behaviour of the experimental total cross section. Therefore, a Landau–Zener model (cf Zener 1932) was assumed to be applicable. The impact-parameter-dependent excitation probability was calculated using the proper molecular wavefunctions of the two coupled states. The total Ag L-excitation cross section was then computed by a numerical integration over all ion trajectories. The DFS potential was used in these calculations. All other couplings were neglected. The Ag L-fluorescence yield was taken from Bambynek *et al* (1972) as $\omega_L \simeq 0{\cdot}055$. The excitation cross section per initial vacancy, $\bar{\sigma}_x$, thus obtained, for the crossing at $R = 0{\cdot}092$ au, is included in figure 2 (chain curve). For ion energies of about 5 MeV, this function passes through a broad maximum. From a comparison of the experimental cross section σ_x and the model cross section $\bar{\sigma}_x$ it follows that the number of initial vacancies $N(v) = \sigma_x/\bar{\sigma}_x$ in the levels feeding the crossing at 0·092 au is about unity just above excitation threshold (v is the ion velocity). We may assume that these vacancies are created in the Ag M shell by a long-range radial coupling on the incoming part of the trajectory (Demkov 1964). As was suggested by Fastrup (1975) and Meyerhof *et al* (1977) for K excitation in slow heavy-atom collisions, we plot $N(v)$ against $1/v$ (insert in figure 2). The resulting dependence is approximately linear within the experimental uncertainty down to ion energies as low as 2 MeV, i.e. $1/v = 0{\cdot}585 \times 10^{-8}\ \mathrm{s\,cm^{-1}}$. Below 2 MeV deviations occur; they are caused by differences between the model cross section $\bar{\sigma}_x$ and the true cross section. An estimate of $N(v)$ below 2 MeV may nevertheless be obtained by extrapolation (full line in the insert). It should be noted that $N(v)$ appears to reach values greater than two for high energies, even though this is the maximum number of vacancies in a σ level. This may in part be caused by the fairly large uncertainty ($\pm 50\%$) in the absolute scale of the experimental total cross sections. In addition, due to the efficient and simultaneous excitation of outer shells in such energetic heavy-ion collisions, the fluorescence yield ω_L may be higher than in neutral atoms. The enhancement, however, should not be large. The energy shifts of the L_α and $L_{\beta 1}$ lines were about 75 and 100 eV (± 30 eV), respectively. This is in agreement with earlier results in similar collision systems (Datz *et al* 1971) and has been explained by the presence of two to four additional M vacancies at the time of L-vacancy decay. Such small additional M excitation is not expected to change ω_L significantly. At much higher ion energies other excitation channels become of importance thus leading to an apparent increase in $N(v)$, e.g., via the crossings at small internuclear separations, or via direct couplings between the molecular L and M levels. In any case, the fluorescence yield as well as additional excitation processes are expected to be only weakly dependent on the ion energy if compared to the sharp rise of the Ag L cross section at about 1 MeV. Thus, they will not influence the shape of the cross section function in the narrow energy regime of interest here; they may, however, be responsible for over-estimating the absolute scale of $N(v)$.

In the energy range investigated, the model Ag L-excitation function in Xe–Ag collisions is then given by $N(v)\bar{\sigma}_x$. For illustration, it is also shown in figure 2 (broken curve). As stated above, the deviations from the experimental curve are due to the shortcomings of the Landau–Zener model: firstly, at and below 1·06 MeV the Landau–Zener cross section vanishes thus underestimating the real value; in addition, the model neglects Coulomb ionisation. Secondly, for trajectories which penetrate to internuclear distances slightly smaller than $R = 0{\cdot}092$ au, the model assumes fully adjusted wavefunctions. Since this is not really the case, the model overestimates the cross sections for ion energies somewhat above 1·06 MeV.

The deviation of the Landau–Zener cross sections from the observed cross sections at threshold indicates the necessity for a more rigorous theoretical treatment. It should be pointed out, however, that no adjustable parameters were used in the calculation of the model cross sections. From this point of view, the agreement between the calculations and the experiment is encouraging; it demonstrates that a detailed experimental check of electron-correlation diagrams should be possible from excitation-threshold measurements even in very heavy collision systems.

Acknowledgment

We are indebted to the technical staff of SUNI for their able assistance with the experiment.

References

Baerends E J, Ellis D E and Roos P 1973 *Chem. Phys.* **2** 41
Bambynek W, Craseman B, Fink R W, Freund H-U, Mark H, Swift C D, Price R E and Venugopala Rao P 1972 *Rev. Mod. Phys.* **44** 716
Datz S, Moak C D, Appleton B R and Carlson T E 1971 *Phys. Rev. Lett.* **27** 363
Demkov Yu N 1964 *Sov. Phys.–JETP* **18** 138
Fastrup B 1975 *Proc. 9th Int. Conf. on Physics of Electronic and Atomic Collisions* ed J S Risley and R Geballe (Seattle: University of Washington Press) p 361
Fricke B, Morović T, Sepp W-D, Rosén A and Ellis D E 1976 *Phys. Lett.* **59A** 375
Lutz H O, McMurray W R, Pretorius R, van Heerden I J, van Reenen R J and Fricke B 1976 *J. Phys. B: Atom. Molec. Phys.* **9** L157
Meyerhof W E, Anholt R and Saylor T K 1977 *Phys. Rev.* A **16** 169
Morović T, Fricke B, Sepp W-D, Rosén A and Ellis D E 1977 *Phys. Lett.* **63A** 12
Zener C 1932 *Proc. R. Soc.* A **137** 696