Observation of Auger transitions in a quasimolecule

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Electrons observed in atomic collisions are attributed to Auger transitions in a quasi-molecular system of two colliding atoms. It is established that the lifetime of the vacancies in the quasi-molecule is comparable with the collision times and amounts to $\sim 10^{-16}$ sec.

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Investigations of x rays produced in radiative transitions in quasimolecules are being diligently investigated of late.[1] It is known at the same time that the lifetimes of vacancies in not very deep electron shells are determined com-

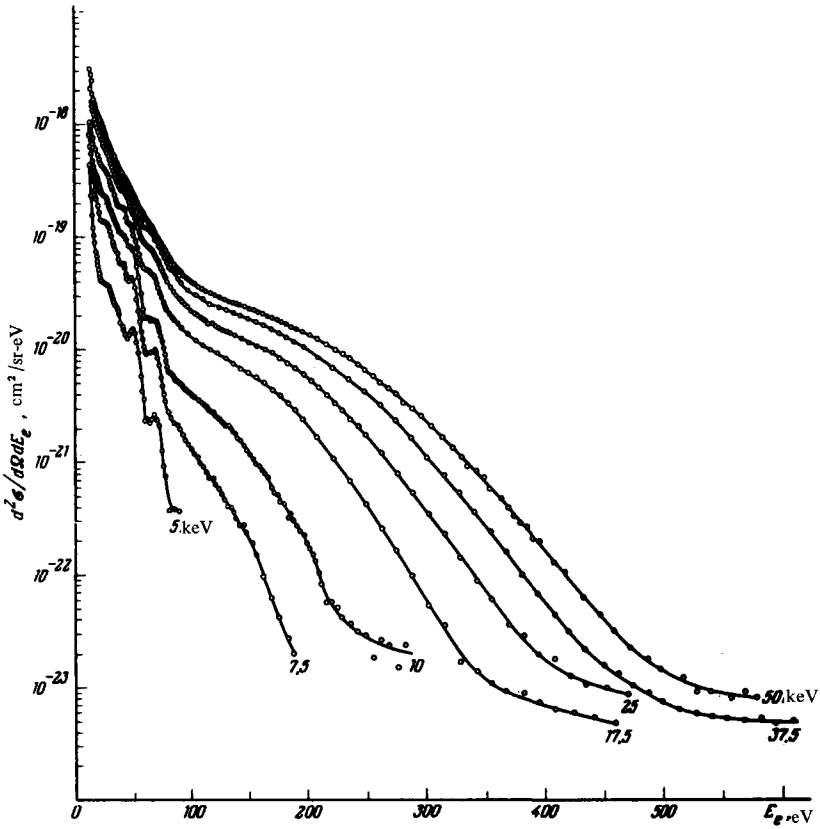

FIG. 1. Energy spectra of electrons produced in $Kr^+ - Kr$ collisions.

pletely by the Auger-transition times. The radiative times as a rule cannot be used to determine the lifetimes of quasi-molecular states, owing to the lack of data on the fluorescence yields of such complicated systems as a quasi-molecule.

We used the procedure of[2] to investigate the energy spectra of electrons produced in $Kr^+ - Kr$ and $Ar^+ - Kr$ collisions. Figure 1 shows the spectra of electrons for $Kr^+ - Kr$ collisions at initial energies E_0 from 5 to 50 keV. A discrete structure is observed in the spectrum, in the electron energy (E_e) interval from 20 to 80 eV, and a broad band is observed at energies above 100 eV.

The discrete lines are connected with Auger transitions to $3d$ vacancies in Kr. The electron peaks with energies from 20 to 60 eV correspond to transitions with participation of $4s$ and $4p$ electrons. The energies of these electrons agree with the energies calculated by Larkins[3] for the corresponding transitions. It is seen from Fig. 2 that the cross section σ_1 for the production of the considered electrons agrees in magnitude and in the dependence on the initial energy with the cross section for the production of $3d$ vacancies, determined from our data on the inelastic energy losses.[4]

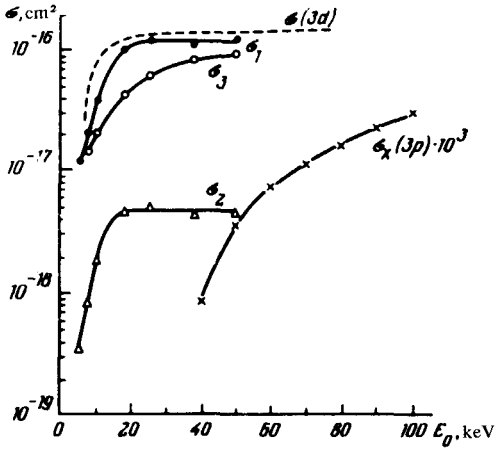

FIG. 2. Cross sections σ_1, σ_2, and σ_3 for the production of different groups of Auger electrons, $\sigma_x(3p)$ for the x-ray emission, and $\sigma(3d)$ for the production of $3d$ vacancies vs the initial energy E_0 for $Kr^+ - Kr$ collisions. (The total cross sections σ_3 were taken into account with allowance for the contribution $(d^2\sigma/d\Omega\, dE_e)(E_e)$ in the region $0 \leq E_e \leq 100$ eV in accordance with the assumption that the band electrons have a quasimolecule origin.)

The peaks at energies from 60 to 80 eV are apparently connected with transitions to $3d$ vacancies from the excited states of the Kr ions. It follows from Fig. 2 that the threshold for the production of these electrons (the cross section σ_2) agrees with the threshold for the production of $3d$ vacancies.

The broad band in the electron spectra cannot be explained with the aid of Auger transitions in the Kr ions. First, the energy of the band electrons greatly exceeds the energy of the transitions to the $3d$ vacancies. Nor can the band be connected with the formation of $3p$ vacancies. It is seen from Fig. 2 that the band excitation threshold (cross section σ_3) differs significantly from the threshold for the formation of $3p$ vacancies, determined from the data of Tawara *et al.* [5] on the x-ray yield.

The band electrons can be attributed to Auger transitions in a quasimolecule. A comparison of the correlation diagram of the $Kr^+ - Kr$ system (Fig. 3) with

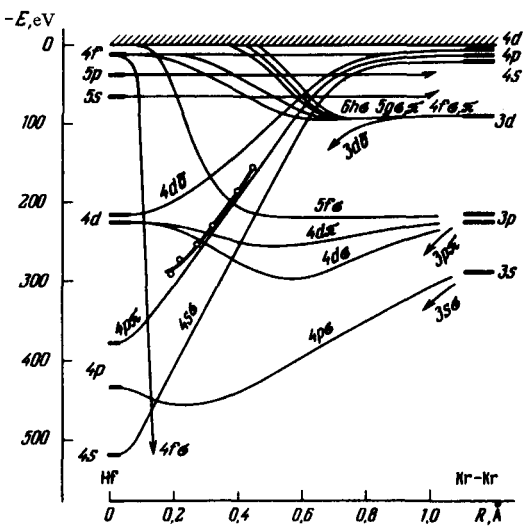

FIG. 3. Correlation diagram of molecular orbitals of the Kr – Kr system. The circles show the course of an orbital obtained from the experimental data.

the energies of the band electrons shows that the band can be connected with transitions to the $4d\delta$ and $4p\pi$ orbitals at small distances between nuclei ($R \lesssim 0.6$ Å). The orbital $4d\delta$ is formed of free $4d$ levels of Kr, and can have four vacancies. The orbital $4p\pi$ is formed of $4p$ levels of Kr. In the case of $Kr^+ - Kr$ collision, there is one vacancy on this level prior to the approach of the particles. The probability of a vacancy appearing on the $4p\pi$ orbital ranges from 1/3 to 2/3, depending on how strongly the $4p$ levels of the Kr ion and atom are coupled under the collision conditions.

To check on the quasimolecule origin of the band, we investigated the electron spectra in $Ar^+ - Kr$ collisions. In this case, the energies of the $4d\delta$ and $4p\pi$ orbitals, in the limit of a unified atom ($R = 0$), are respectively ~60 eV and ~140 eV. Indeed, in the $Ar^+ - Kr$ collision, $E_0 = 25$ keV, the electrons that can be connected with transitions in the quasimolecule have energies significantly lower than the energies of the molecular-orbital (MO) electrons in $Kr^+ - Kr$ collisions.

The experimental data can be used to determine the energy $E(R)$ of the orbital and the probability $W(R)$ of the vacancy decay. The maximum electron energy in the band, at a fixed initial energy E_0, corresponds to transitions at the minimal internuclear distances R_0 attainable in such collisions. The experimental MO, determined accurate to the binding energy of the outer electrons, is shown in Fig. 3. If transitions to several orbitals are possible in the quasimolecule, then our procedure makes it possible to find the molecular orbital with the maximum energy. Indeed, the experimental molecular orbital is close to the $4p\pi$ orbital.

The differential cross section for the production of molecular orbitals of electrons can be written in the form

$$\frac{d\sigma}{dE_e} = fW(R)\frac{dR}{dE_e}\int_0^{p_0(R)} \frac{2\pi p\,dp}{v_R(p)} \exp\left(-\int_R^{R_x} \frac{W(R')dR'}{v_{R'}(p)}\right)\left[1+\exp\left(-2\int_{R_0}^{R} \frac{W(R')dR'}{v_{R'}(p)}\right)\right],$$

where f is the initial number of vacancies on the orbital, $W(R)$ is the decay probability, R_x is the largest internuclear distance at which an Auger transition is possible, p is the impact parameter, $p_0(R)$ is the impact parameter at which R is the turning point, and v_R is the radial velocity. Assuming $W(R)$ to be constant in the interval $0 \leq R \leq R_x$ and using $E(R)$ for the experimental molecular orbital, we have integrated $d\sigma/dE_e$ numerically and obtained $f = 0.4$—4 and $W = (0.5$—$3) \times 10^{16}$ sec^{-1}. In the initial-energy interval investigated by us, the vacancy lifetime in the molecule turned out to be comparable with the collision time, and much less (by approximately two orders of magnitude) than the lifetime of the vacancies in isolated atoms.

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