THE ANGULAR DISTRIBUTION OF THE $KL\text{-}LL_{2,3}L_{2,3}$ SATELLITE AUGER TRANSITIONS IN Ne

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Recently [1,2] the angular distributions of Auger electrons arising from the decay of double-vacancy states in Ne were measured for the first time. The doubly ionised Ne atoms were produced in collisions of 5.5 MeV/a.m.u. Ne^{3+} ions with Ne atoms. The K Auger spectrum was studied in the 782-805 eV energy range, where apart from the $K\text{-}L_1L_{2,3}(^3P)$ and $K\text{-}L_{2,3}L_{2,3}(^1S, ^1D)$ diagram lines there were satellite lines arising from the decay of doubly ionised neon atoms, namely the $KL\text{-}LL_{2,3}L_{2,3}$ satellite transitions, where one of the initial vacancies (K) decayed and the other (L) was a "spectator".

In heavy ion-atom collisions production of several vacancies in electron shells is highly probable. Therefore, the intensities of the $KL\text{-}LL_{2,3}L_{2,3}$ satellites are of the same order of magnitude as those of diagram lines or even greater. This facilitates the measurement of the angular distribution of satellite lines.

Investigations of the angular distribution of satellite lines in the Auger spectrum started by Ricz et al. [1,2] are of interest for two reasons. Firstly, the satellite spectrum is in general very complicated and conventional data used for the identification of lines (transition energies and line intensities) may be insufficient. For example, in the energy region considered the energy separation of two neighbouring peaks is 1 to 3 eV. However, the majority of existing theoretical methods give the line energy with an accuracy not better than several electronvolts. It is obvious that in such a case it is easy to make a mistake. Comparison of line intensities involves difficulties because it is necessary to know the initial population of highly excited states with two and more vacancies produced in ion-atom collisions, which in itself is an intricate theoretical problem. Measurement of the angular distributions gives additional information which can help to identify lines since, as will be seen from the following, different lines have, in general, very different anisotropy the angular distribution. Secondly, the study of the angular dis-ibution of satellite lines of the Auger spectrum is of independent terest because it allows one to obtain new information on the ato-c electron shell, such as the interaction of vacancies in the atom, ectronic state relaxation in the presence of holes in some sub-ells, etc.

In the present paper the results of theoretical study of the -$LL_{2,3}L_{2,3}$ satellites in Ne are presented. As far as we know, in e literature there are no other theoretical studies of the angular stribution of satellite Auger transitions. We have calculated the gular distribution coefficients, relative intensities and energies satellite lines.

First consider the angular distribution. As has already been men-oned, in the 782-805 eV energy range there are diagram lines cor-sponding to the K-vacancy decay. According to the general theory], their angular distribution must be isotropic, which was confir-d by the experiment [1,2]. The satellite spectrum in this energy gion is rather simple and contains six lines arising from the fol-wing transitions

$1s^{-1}2s^{-1}(^1S) - 2s^{-1}2p^{-2}(^2D)\ q$ [116 pp (^1S - ^2D)]
$1s^{-1}2s^{-1}(^3S) - 2s^{-1}2p^{-2}(^2D)\ q$ [116 pp (^3S - ^2D)]
$1s^{-1}2p^{-1}(^1P) - 2p^{-3}(^2D)\ q$ [125 pp (^1P - ^2D)]
$1s^{-1}2p^{-1}(^3P) - 2p^{-3}(^2D)\ q$ [125 pp (^3P - ^2D)]
$1s^{-1}2p^{-1}(^1P) - 2p^{-3}(^2P)\ q$ [125 pp (^3P - ^2P)]
$1s^{-1}2p^{-1}(^3P) - 2p^{-3}(^2P)\ q$ [125 pp (^3P - ^2P)]

the following we shall use the notation of lines which is given square brackets.

The unpolarised beams of atoms and ions were used in the experi-ent [1,2]. In this case the angular distribution of Auger line in-nsity is determined by the expression [3]

$$I(\theta)=\frac{I_0}{4\pi}\left(1+\sum_{k=2,4,\dots}\alpha_k \mathcal{A}_{k0} P_k(\cos\theta)\right) \qquad (1)$$

here I_o is the total intensity of the line, α_k are the anisotropy arameters depending, in general, on the Auger decay amplitudes, $\mathcal{A}_{ko}$ naracterise the alignment of the initial excited state, produced in ion-atom collision, P_k ($\cos\theta$) are the Legendre polynomials and θ is the angle between the initial ionic beam direction and the di-ection of Auger electron.

In order to obtain the anisotropy coefficients a_2 for the two
ansitions $125pp(^{1,3}P-^2P)$, it is necessary to calculate the parame-
rs α_2 which depend on the Auger decay amplitudes since in these
ansitions electrons with different orbital angular momenta may be
itted (s and d electrons).

The Auger decay amplitudes were calculated in the independent par-
le approximation. For calculating the Coulomb matrix elements in-
ved we used the Hartree-Fock wave functions. The additional L-va-
cy in the initial and final states was taken into account in the
lowing way. The wave functions of the vacancies involved in the
er decay were determined in the field of the L-hole which acted as
spectator". The wave function of the Auger electron was found in
field of a triply ionised atom. Such determination of the single
tron wave functions corresponds to the inclusion of a certain
of many-electron interactions [4].

Table 1

The energies, relative intensities and angular anisotropy
parameters of the $KL-LL_{2,3}L_{2,3}$ transitions in Ne

ransition	E (eV)		I		a_2	
	exper. [2]	theory	exper. [1]	theory	exper. [2]	theory
$p(^3P - ^2P)$	783.19	783.4	0.304	0.324	0.11 (3)	0.15
$p(^3P - ^2D)$	785.49	787.1	0.547	0.693	-0.07 (4)	-0.18
$p(^3S - ^2D)$	785.97	787.8	0.297	0.294	-0.15 (7)	0.00
$p(^1P - ^2P)$	787.55	787.6	0.139	0.108	0.08 (6)	0.15
$p(^1P - ^2D)$	790.29	791.2	0.231	0.231	-0.18 (3)	-0.18
$p(^1S - ^2D)$	792.21	795.9	0.072	0.098	0.00 (6)	0.00

s is seen from Table 1, the calculated values of the anisotropy
ficients agree well with the experimental data. Exceptions are
transitions $125pp(^3P - ^2D)$ and $116pp(^3S - ^2D)$, which belong to
experimentally unresolved doublet. In our model the transition
$p(^3S - ^2D)$ should be isotropic (see above), whereas experiment
s a large anisotropy [2]. On the contrary, according to the cal-
tions, the transition $125pp(^3P - ^2D)$ should be nonisotropic,
eas in the experiment [2] it is practically isotropic. Ricz et al.
pointed out the uncertainty in the decomposition procedure for
unresolved doublet and the resulting ambiguity of identification.
w analysis of the experimental data seems to be desirable with

the inclusion of the restrictions imposed by the angular distribution properties.

It is interesting to compare the theoretical and experimental anisotropy for the unresolved doublet. The average anisotropy of a doublet is

$$\tilde{a}_2 = \frac{I_0^{(1)} a_2^{(1)} + I_0^{(2)} a_2^{(2)}}{I_0^{(1)} + I_0^{(2)}}$$

where I_0 is the intensity and a_2 is the anisotropy coefficient of the line. The superscripts (1) and (2) refer to the lines $125pp(^3P-^2D)$ and $116pp(^3S-^2D)$. Using the published data [1,2], one can obtain the following anisotropy coefficient for the doublet $\tilde{a}_2 = -0.108$. The corresponding theoretical value $\tilde{a}_2 = -0.127$ agrees fairly well with the experimental one, therefore, our simple model is not inconsistent with the experiment.

Table 1 lists the energies of the satellite Auger transitions. They were determined as the difference of the total Hartree-Fock energies of doubly and triply ionised atoms. Ion energies were calculated by solving self-consistently the system of the Hartree-Fock equations for the initial two-hole state and final three-hole state separately. This procedure allows one to partly take into account the effects of interaction of the vacancies, hole relaxation, etc. [4]. The energies of the satellite lines found in this way agree fairly well with the experimental results [1,2]. The discrepancy is 1 to 3 eV.

We have also calculated the relative line intensities. The double-vacancy state populations were determined as follows. Suppose that the probabilities q_n of production of $\underline{n}$ vacancies in the L-shell (in addition to the K-vacancy) have the binomial distribution

$$q_n = \sum_{i+k=n} C_2^i p_s^i (1-p_s)^{2-i} C_6^k p_p^k (1-p_p)^{6-k} \qquad (4)$$

where C_m^k is the number of combinations of k electrons chosen from a set of m. The ratio p_p/p_s of the ionisation probabilities of the $L_{2,3}$ and L_1 subshells is known from the analysis of experiment [5] to be 1.57. Using this value, expression (4) and the calculated amplitudes of Auger decay, we calculated the relative intensities of the satellite lines. For comparison with the experiment we normalise our results to the intensity of the $125pp(^1P-^2D)$ line. The relative intensities thus obtained agree satisfactorily with the experimental data (see Table 1).

Comparison of the results of our calculations and experiment [1,2] hows that the simple model used in this work gives rather a good escription of various experimental data. The only exception is the gular distribution of the 116pp($^3S-^2D$) and 125pp($^3P-^2D$) doublet, r which an additional analysis is needed.

Further investigations of the angular distribution of the satel-te Auger lines, in our opinion, appear to be very interesting and eful especially for the problem of identification of lines in com-ex spectra.

References

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