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<tr>
<td>Citation</td>
<td>Bulletin of the Institute for Chemical Research, Kyoto University (1982), 60(5-6): 289-293</td>
</tr>
<tr>
<td>Issue Date</td>
<td>1982-11-15</td>
</tr>
<tr>
<td>URL</td>
<td><a href="http://hdl.handle.net/2433/77012">http://hdl.handle.net/2433/77012</a></td>
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<tr>
<td>Type</td>
<td>Departmental Bulletin Paper</td>
</tr>
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<td>Textversion</td>
<td>publisher</td>
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ZT-oscillation of Electron Capture Cross Sections of MeV Helium Ions*

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Received March 30, 1982

By taking account of the atomic shell structures, electron capture cross sections of He5+ ions for various target atoms (ZT=1–90) are calculated with the Bohr-Lindhard model and are found to oscillate with Zr. Experimentally-observed ZT-oscillation of equilibrium mean charges is reproduced satisfactorily by using these cross sections.

I. INTRODUCTION

In recent years much effort have been made for the study of charge changing collisions involving multicharged ions and heavy target atoms intending to the practical applications to the thermonuclear fusion researches. We have measured equilibrium mean charges of helium ions over the wide range of target atoms by the method of backscattering from solid targets.1,2) These solid data together with gas data3-5) show oscillatory behaviour as a function of target atomic number Zr. This oscillation is probably caused by the characteristic of capture cross sections, since electron capture from target atoms depends strongly on the target shell structures.

Most of theoretical studies on electron capture, however, have been limited to the simplest cases such as hydrogen or helium like target atoms.6) In this paper, we have calculated the single electron capture cross sections ε21 by He2+ ions from various target atoms with ZT=1–90 at the incident energies 1 and 2 MeV. Calculations are made on the basis of the Bohr-Lindhard classical model7) which is simple and gives us a clear physical picture for the capture process.

The equilibrium mean charges of helium ions have been estimated with the above electron capture cross sections and with electron loss cross sections which are assumed to have monotonic dependence on Zr.

II. CALCULATIONS OF ELECTRON CAPTURE CROSS SECTIONS

In the Bohr-Lindhard model, the following two characteristic distances between a projectile ion and a target atom are introduced to explain the electron capture process. One is the electron release distance Rr where the exerted force on a target

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* This paper was accepted on the occasion of the retirement of Prof. emeritus T. Yanabu and is dedicated to him.

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electron by the projectile ion is equal to the atomic binding force for that electron. Another is the electron capture distance $R_e$ where the released electron can be captured by the projectile. For simplicity the released electron is assumed not to have velocity relative to the target nucleus, and therefore, velocity of this electron relative to the projectile is the same as the projectile velocity $V$. These two distances are determined by the following relations;

$$q_e^2/R_e^2 = mu^2/r, \quad (1)$$
$$q_e^2/R_e = mV^2/2, \quad (2)$$

where, $q_e$ the charge of the projectile ion, $m$ the electron mass, $u$ and $r$ the orbital velocity and radius of the electron under consideration. The capture cross section is given in the first approximation by $\pi R_e^2$ for $R_e < R_e$ and zero for $R_e > R_e$. Since the electron release is a gradual process and requires a time-duration of the order of magnitude $r/u$, the projectile can capture the released electron if the projectile approaches up to $R_e$ during this time. By introducing capture probability of the released electron, $\epsilon$, and the corrected factor for the time-duration, $\alpha$, capture cross sections are expressed more exactly as follows;

$$\sigma_1 = \pi \alpha R_e^2 = \pi \alpha a_0^2 q(r/a_0) (v_0/u)^2, \quad \text{for} \quad R_e < R_e \quad (3)$$
$$\sigma_{11} = \pi \alpha R_e^2 \beta(u/r) (R_e/V) = \epsilon \beta \alpha \pi a_0^2 q^2(a_0 | r) (u/v_0) (v_0/V), \quad \text{for} \quad R_e > R_e \quad (4)$$

where $a_0$ and $v_0$ are Bohr radius and Bohr velocity, respectively. In the following calculations, $\epsilon$ and $\beta$ are taken as fitting parameters. The total cross section is obtained by summing contributions of all target electrons,

$$\sigma_{\text{total}} = \sum_i \sigma_i(u_i, r_i) N_i, \quad \text{with} \quad k = \text{I or II} \quad (5)$$

where $r_i$, $u_i$ and $N_i$ are orbital radius, velocity and number of electrons in the $i$-th subshell of target atom. Instead of this discrete summation, Knudsen et al \cite{Knudsen1958} calculated by integrating over $u$ in terms of relations $dN = Z_T^{1/3} du/v_0$ and $r = a_0 Z_T^{1/3} v_0/u$ obtained from the Bohr's statistical atomic model. As can be expected, their cross sections show only averaged $Z_T$ dependence, giving no oscillatory structure. In this paper, the summation of Eq. (5) have been carried out with the orbital velocity $u_i$ calculated from the binding energy \cite{Itoh1968} $E_i = m u_i^2/2$ and the radius $r_i$ determined from the maximum radial density of the wave function. \cite{Itoh1970}

As an typical example, calculated cross sections with $(\epsilon, \beta) = (1, 1)$ for the collision system $\text{He}^{2+} + \text{Ar} \rightarrow \text{He}^+ + \text{Ar}^+$ are compared with other experimental data \cite{Hargreaves1968} in Fig. 1. There are discrepancies between $\sigma_1$ and $\sigma_{11}$ at the critical projectile velocities giving $R_e > R_e$. In order to connect two cross sections smoothly, the critical velocities were shifted to the crossing points of these cross sections in such ways as shown by dashed lines in this figure.

In Fig. 2, are shown the $Z_T$ dependence of cross sections $\sigma_{21}$ for 1 MeV $\text{He}^{2+}$ with two sets of fitting parameters $(\epsilon, \beta) = (1, 1)$ and $(0.5, 4)$. They show clearly oscillatory behaviour. By changing two parameters $\epsilon (<1)$ and $\beta (>1)$, peaks of cross sections shift to lower $Z_T$.

Fig. 3 shows the $Z_T$ oscillations for two different projectile energies 1 and 2 MeV, with $(\epsilon, \beta) = (0.5, 4)$. The experimental data \cite{Hargreaves1968} for 1 MeV are also plotted in this figure. Present calculations are in fairly good agreement with them. For 2 MeV projectile, contributions of each subshells are drawn by dashed curves. They
show that the oscillation is due to the dominant contributions of the specified subshell electrons which have orbital velocities comparable to the projectile velocity. This is just the suggestion given by Bohr-Lindhard. This “velocity matching” is verified more directly by using Brinkman-Krammers approximation. When hydrogenic wave functions are used for the electrons under consideration, BK approximation gives simple analytic formula\(^{16}\) for capture cross section for the electron from \(i\)-th shell of the target atom into \(n\)-th shell of the projectile.

\[
\sigma_{\text{BK}} = \frac{218}{15} \pi a_0^2 n^2 (I_i I_n)^{5/2} (\nu_0/V)^2 [\langle V/\nu_0 \rangle + (I_i - I_n) (\nu_0/V)]^2 + 4I_n^{-5},
\]

(6)
where $I_i$ and $I_n$ are average binding energies (in unit of Rydberg energy) for the shell with principal quantum number $i$ and $n$ of the target atom and projectile ion, respectively. Solving equation $\frac{\partial \sigma_{KI}}{\partial I_i} = 0$, we can obtain the optimum orbital velocity of electron which is most easily captured for given projectile velocity $V$, that is, $u_t = V/\sqrt{3}$, for $I_i > I_n$. 

This relation indicates that target electron with velocity $u = 0.6V$ contribute most dominantly to the capture process. In Fig. 3, we can see that peaks at $Z_T = 2-3, 11, 33, 55$ and $74$ for 1 MeV projectile shift to $Z_T = 4, 15, 38, 67$ and $87$ for 2 MeV.

III. EQUILIBRIUM MEAN CHARGE

In the helium beams with energies above 1 MeV, the equilibrium neutral fraction is negligibly small ($<0.01$). Then, the mean charge $\bar{q}$ can be estimated by the formula $\bar{q} = (\sigma_{21} + 2\sigma_{12}) / (\sigma_{21} + \sigma_{12})$. For the capture cross section $\sigma_{21}$, theoretical values taken from Fig. 3 can be used. For the loss cross section $\sigma_{12}$, the empirical values can be estimated by connecting experimental loss cross sections with smooth and monotonous curves as shown in Fig. 4. Mean charges of helium ions at energies 1 and 2 MeV calculated with these cross sections are shown in Fig. 5, where experimental gas and solid data at 1 MeV are also shown. Theoretical results agree very well with experimental ones over the wide range of target atoms. Discrepancies in the range $Z_T > 70$ would be attributed to the incorrect values of fitting parameters which should be different from those for lighter atoms due to the complexity of electronic structure of heavier atoms.
IV. CONCLUSIONS

The single electron capture cross sections of He\(^{2+}\) ions for target atoms \(Z_T = 1-90\) have been calculated with Bohr-Lindhard classical model. By calculating the individual subshell contributions, \(Z_T\)-oscillations was obtained. Cross section peaks are found to shift to higher \(Z_T\) as the ion velocity increases. From the simple BK calculations, we found that electrons with velocity \(= 0.6V\) contribute most dominantly to the capture process. Experimentally-observed \(Z_T\)-oscillation of equilibrium mean charge was reproduced very well with the calculated capture cross sections and experimentally-determined smooth curve of loss cross sections. However, there remains a problem whether the loss cross sections have really no \(Z_T\)-oscillation. In order to make assure directly the \(Z_T\)-oscillation, more precise experimental works should be made on the loss and capture cross sections over the wide range of \(Z_T\).

More rigorous calculations were made recently by Dmitriev et al\(^{20}\) with BK approximation and by Kaneko et al\(^{21}\) with two-state-two-center model, giving similar \(Z_T\)-oscillation to ours.

ACKNOWLEDGEMENTS

We are grateful to professor M. Sakisaka and Dr. M. Tomita for continuous supports and encouragements in the course of this work. The support from Japan Society for the Promotion of Science to one of us (A. I.) is also gratefully acknowledged.

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