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Z_T-oscillation of Electron Capture Cross Sections of MeV Helium Ions‡

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By taking account of the atomic shell structures, electron capture cross sections of He^{2+} ions for various target atoms ($Z_T=1$–90) are calculated with the Bohr-Lindhard model and are found to oscillate with Z_T. Experimentally-observed Z_T-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 data[3~5] show oscillatory behaviour as a function of target atomic number Z_T. 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 σ_{21} by He^{2+} ions from various target atoms with $Z_T=1$–90 at the incident energies 1 and 2 MeV. Calculations are made on the basis of the Bohr-Lindhard classical model[7] 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 Z_T.

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 R_r where the exerted force on a target

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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_c 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;

$$qe^2/R_r^2 = mu^2/r, \tag{1}$$

$$qe^2/R_c = mV^2/2, \tag{2}$$

where, qe 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 πR_r^2 for $R_r < R_c$ and zero for $R_r > R_c$. 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_c during this time. By introducing capture probability of the released electron, ε, and the correcting factor for the time-duration, β, capture cross sections are expressed more exactly as follows;

$$\sigma_{\mathrm{I}} = \varepsilon\pi R_r^2 = \varepsilon\pi a_0^2 q(r/a_0)(v_0/u)^2, \text{ for } R_r < R_c \tag{3}$$

$$\sigma_{\mathrm{II}} = \varepsilon\pi R_c^2 \beta(u/r)(R_c/V) = \varepsilon\beta 8\pi a_0^2 q^3 (a_0/r)(u/v_0)(v_0/V)^7, \text{ for } R_r > R_c \tag{4}$$

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

$$\sigma_{q,q-1} = \sum_i \sigma_k(u_i, r_i) N_i, \text{ with } k = \mathrm{I} \text{ or } \mathrm{II} \tag{5}$$

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*[8] 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[9] $I_i(=mu_i^2/2)$ and the radius r_i determined from the maximum radial density of the wave function.[10]

As an typical example, calculated cross sections with $(\varepsilon, \beta) = (1, 1)$ for the collision system $He^{2+} + Ar \rightarrow He^{+} + Ar^{+}$ are compared with other experimental data[11] in Fig. 1. There are discrepancies between σ_I and σ_{II} at the critical projectile velocities giving $R_r = R_c$. 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 σ_{21} for 1 MeV He^{2+} with two sets of fitting parameters $(\varepsilon, \beta) = (1, 1)$ and $(0.5, 4)$. They show clearly oscillatory behaviour. By changing two parameters $\varepsilon(<1)$ 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 $(\varepsilon, \beta) = (0.5, 4)$. The experimental data[12~15] 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

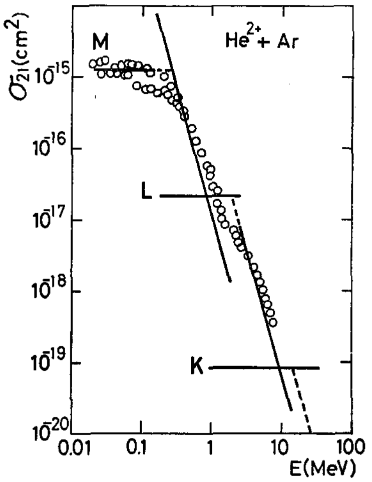

Fig. 1. Capture cross sections σ_{21} as a function of projectile energy E for $He^{2+}+Ar \rightarrow He^{+}+Ar^{+}$. Solid lines are theoretical and open circles are experimental.[11]

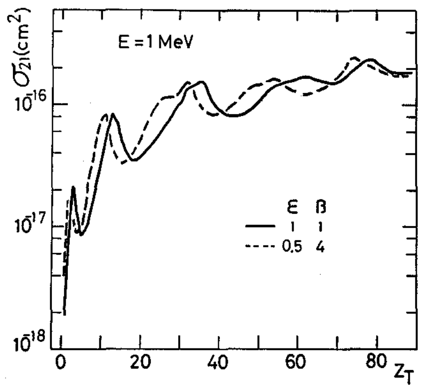

Fig. 2. Z_T-oscillation of capture cross sections σ_{21} for 1 MeV He^{2+} projectile. Dependence on parameters ε and β.

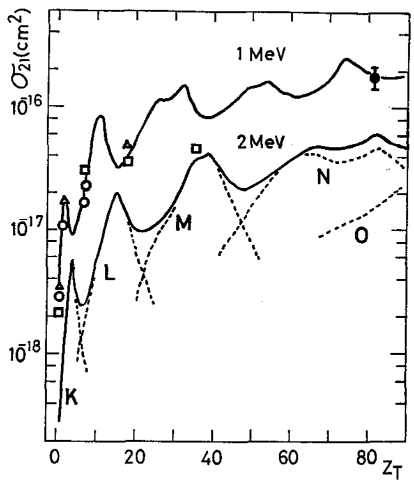

Fig. 3. Z_T-oscillation of capture cross sections σ_{21} for 1 and 2 MeV He^{2+} projectile. Experimental; □ (ref. 12), △ (ref. 13), ○ (ref. 14), ● (ref. 15). Experimental values for H, N and O are one-half of their molecular data.

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.[7] 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.

$$\sigma_{BK}=\frac{2^{18}}{15}\pi a_0^2 n^2 (I_i I_n)^{5/2}(v_0/V)^2[((V/v_0)+(I_i-I_n)(v_0/V))^2+4I_n]^{-5}, \quad (6)$$

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 $\partial\sigma_{BK}/\partial I_i=0$, we can obtain the optimum orbital velocity of electron which is most easily captured for given projectile velocity V, that is,

$$u_i=V/\sqrt{3}, \text{ for } I_i \gg I_n. \tag{7}$$

This relation indicates that target electron with velocity $u \simeq 0.6V$ 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).[5] 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 σ_{21}, theoretical values taken from Fig. 3 can be used. For the loss cross section σ_{12}, the empirical values can be estimated by connecting experimental loss cross sections[4,15,17~19] with

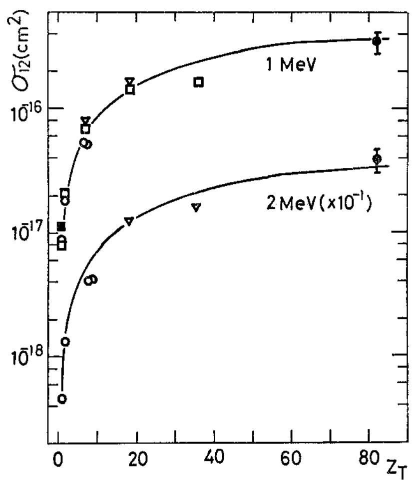

Fig. 4. Loss cross sections σ_{12} for 1 and 2 MeV He^+ projectile. Solid curves are drawn by connecting smoothly the experimental values; □ (ref. 4), ● (ref. 15), ▽ (ref. 17), ■ (ref. 18), ○ (ref. 19). Experimental values for H, N and O are one-half of their molecular data.

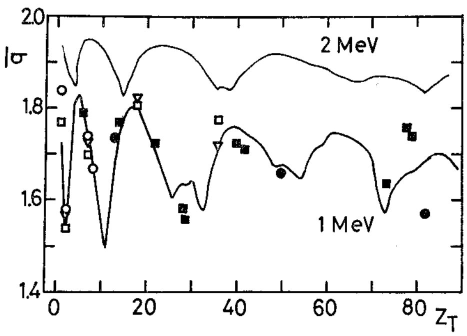

Fig. 5. Equilibrium mean charges $\bar{q}$ of 1 and 2 MeV helium ions. Solid curves are theoretical. Experimental gas and solid data for 1 MeV projectile are represented by open and closed symbols, respectively; ▽ (ref. 3), □ (ref. 4), ○ (ref. 5), ■ (ref. 1), ● (ref. 2).

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[3~5] and solid[1,2] 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.

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