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# Proton and α-particle impact $M$-shell ionization of atoms in binary encounter approximation

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**Abstract.** $M$-shell ionization cross sections for atoms due to the impact of proton and α-particles have been calculated in the binary encounter approximation. The effects of Coulomb deflection of the incident projectile and increase in binding of the target electron have been investigated. Roothan-Hartree-Fock velocity distribution for the target electrons has been used in the present work. The calculated cross-sections have been compared with experimental results and other theoretical calculations wherever available. The present calculations give a good account of experimental observations.

**Keywords.** $M$-shell; ionization cross-section; Coulomb deflection; binding energy correlation; Roothan-Hartree-Fock velocity distribution.

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## 1. Introduction

Investigation of inner-shell ionization of atoms by the impact of heavy charged particles has gained much practical importance, especially, because of the direct use of the particle induced X-ray analysis in many applied fields (Gowda and Powers 1985). $M$-shell studies (theoretical as well as experimental) are scarce in literature (Ishii *et al* 1975; Busch *et al* 1973; Sera *et al* 1980) as compared to the study of $K$- and $L$-shell vacancy production. This is because of the fact that $M$-shell itself is complex in nature (Chen *et al* 1983).

In plane wave Born Approximation (PWBA), Choi (1973) and Johnson *et al* (1979) calculated proton impact inner-shell ionization cross-sections which finally resulted in scaled universal functions for 3*s*, 3*p* and 3*d*. In both the calculations in PWBA, only the effect of Coulomb deflection has been taken into account. Mehta *et al* (1982) have used the PWBA universal function for the direct Coulomb ionization and added to it Oppenheimer Brinkmann Kramers (OBK) results for electron capture by Nikolaev (1967) to calculate $M$-shell X-ray production cross-section. Calculations were also performed by Mehta *et al* (1982) in the perturbed stationary state theory of Brandt and Lapicki (1979). The so-called ECPSSR calculations account for the energy loss and Coulomb deflection of the projectile and the effect of relativistic nature of $M$-shell electron. The ECPSSR calculation goes beyond the first Born approximation which does not include all these effects. Chen *et al* (1983) have scaled their relativistic Dirac-Hartree-Slater calculations of $L$-shell ionization cross-sections to obtain $M$-shell cross-sections.

In recent past, Shrivastava and Roy (1986) have discussed in detail the limitations of quantal as well as BEA scalings. They have concluded that it would not be possible to obtain accurate cross-sections for different shells of different systems due to impact of different projectiles from scaled universal curves. These curves do not incorporate correctly the different physical processes (especially binding energy correction and the effect of wave function) contributing to inner-shell ionization due to heavy particle impact.

Previous results for $K$- and $L$-shell ionization in the BEA (Shrivastava *et al* 1984; Shrivastava and Roy 1986; Chatterjee and Roy 1986) have been found to agree well with the experiments. In case of $M$-shell also, even the BEA scaled results of Garcia (1970) and Garcia *et al* (1973) provide better agreement with the experimental results than those of SCA and PWBA (Thornton *et al* 1974). Keeping in view of the limitations of different scalings and satisfactory agreement of the BEA with experimental observations, we have considered it worthwhile to calculate the $M$-shell ionization cross-sections of atoms due to proton and $\alpha$-particle impact in the binary encounter approximation. We have incorporated the effects of Coulomb deflection of the projectile in the field of target nucleus and increase in binding of the target electron in the presence of the projectile.

## 2. Theoretical considerations

Following Thomas and Garcia (1969) we have incorporated the effect of the Coulomb interaction between the positively charged projectile and the nucleus analytically through the relation (see Shrivastava *et al* 1984).

$$\sigma(E_1) = \sigma(E_1')\left[\frac{1}{2}+\frac{1}{2}\left(1-\frac{Z_1 Z_{2M} e^2}{E_1 a_{2M}}\right)^{1/2}\right]^2, \tag{1}$$

where $\sigma(E_1')$ is the ionization cross-section at the reduced energy

$$E_1' = E_1 - \frac{Z_1 Z_{2M} e^2}{a_{2M}},$$

and

$$Z_{2M} = Z_2 - S_{2M},$$

$Z_1$ and $Z_2$ are the nuclear charges of the projectile and of the target under consideration respectively, $a_{2M}$ and $S_{2M}$ are the radius and the screening constant for the $M$-shell respectively.

The binding energy of an atomic electron is increased due to the presence of slow charged projectile in the vicinity of the nucleus during the collision. This perturbation of the target atomic states by the projectile leads to a reduction in ionization probability. Brandt and Lapicki (1979) have considered that increase in binding occurs as the target electron assumes the binding energy of a united atom of atomic number $(Z_1 + Z_2)$ formed during the collision. To take this increase in binding into account, we have used the $M$-shell binding energy of the united atom $(UZ_1 + Z_2)$ in the present calculations (see also Chen *et al* 1983).

Vriens' (1967) experessions for ionization cross-section incorporating the contributions of the above mentioned effects can be written as,

$$Q(s,t)=\frac{(s+s')^2Z_1^2}{s^2s'^2U_{Z_1+Z_2}^2}\left(1+\frac{2t^2}{3}-\frac{1}{4(s'^2-t^2)}\right)(\pi a_0^2),\quad 1\leqslant 4s'(s'-t)$$

$$=\frac{(s+s')^2Z_1^2}{2s^2s'^2U_{Z_1+Z_2}^2t}\left[\frac{1}{4(s'-t)}+t+\frac{2}{3}\{2s'^3+t^3-(1+t^2)^{3/2}\}\right](\pi a_0^2),$$

$$4s'(s'-t)\leqslant 1\leqslant 4s'(s'+t)$$

$$=0,\quad 1\geqslant 4s'(s'+t). \tag{2}$$

The dimensionless variables can be defined as

$$t^2=v_{2M}^2/v_0^2.$$

$$s^2=v_1^2/v_0^2.$$

and

$$s'^2=s^2-(1{\cdot}058Z_1Z_{2M})/(1836Ma_{2M}UZ_1+Z_2).$$

$v_0^2$ is the corrected ionization energy in rydberg of the shell under consideration. $v_1$, $v_{2M}$ and $M$ (mass of the projectile) are expressed in atomic units.

Finally, the expressions in (2) have been integrated over the Roothan-Hartree-Fock velocity distribution for the target electron. The Roothan-Hartree-Fock radial functions (McLean and McLean 1981) have been used to construct momentum distribution function for the target electrons (see Kumar and Roy 1978).

In accordance with the spin-orbit interaction consideration, we have taken contributions from all the five sub-shells of the $M$-shell of the atomic system, the number of electrons in each sub-shell being determined by the multiplicity $(2J+1)$. The binding energy of each shell, the screening constants and radii of sub-shells have been taken from the tables of Lotz (1968), Fischer (1973) and McLean and McLean (1981), respectively.

## 3. Results and discussion

$M$-shell ionization cross-sections for some atomic systems due to impact of protons and $\alpha$-particles have been calculated along the lines discussed in §2 in the energy region 0·5—50 MeV. The experimental $M$-shell ionization cross-sections $(\sigma_I)$ have been determined from X-ray production cross-sections $(\sigma_x)$ using

$$\sigma_I=\sigma_x/\bar{\omega}_m$$

where $\bar{\omega}_m$ is the average fluorescence yield of the atomic $M$-shell. The values of $\bar{\omega}_m$ for the systems undertaken have been taken from Bambynek *et al* (1972). We have compared the results with the experimental observations and other theoretical calculations wherever available.

Proton impact $M$-shell ionization cross-sections for Au are presented in figure 1. Our calculated cross-sections (including Coulomb deflection and increase in binding) are always within a factor of 1·5 from the experimental values. The present results are in better agreement with the experiments of Mehta *et al* (1982) in the energy range

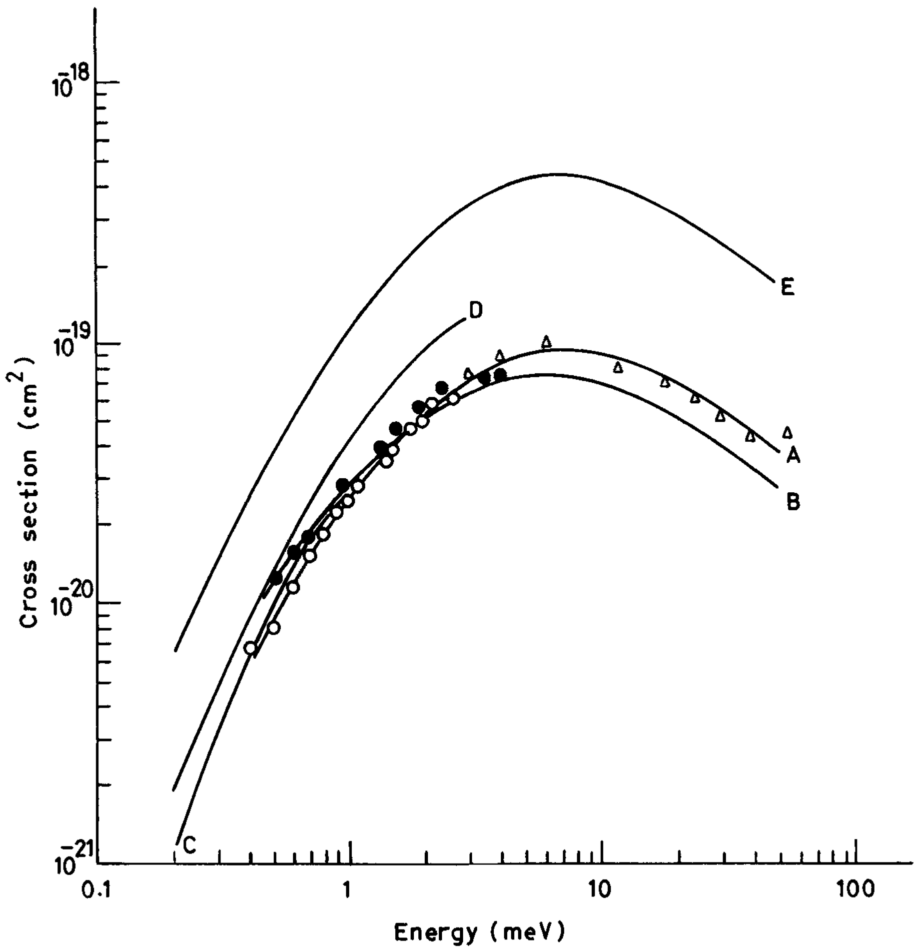


**Figure 1.** Proton impact *M*-shell ionization cross-sections of Au; (A) Present calculation including Coulomb deflection and increase in binding; (B) Present calculation including only increase in binding; (C) Calculation of Chen *et al* (1983); (D) ECPSSR calculation of Mehta *et al* (1982); (E) Scaled PWBA results of Johnson *et al* (1979); ● Experiment (Faria *et al* 1983); ○ Experiment (Mehta *et al* 1982); △ Experiment (Sera *et al* 1980).

up to 1 MeV, whereas the relativistic calculations (up to 1 MeV) of Chen *et al* (1983) in PWBA incorporating the effects of the increase in binding and Coulomb deflection are in better agreement with the experimental observations of Faria *et al* (1983). The agreement of our cross-sections with all the experimental observations is better than the ECPSSR cross-sections of Mehta *et al* (1982) and the scaled plane wave Born cross-sections of Johnson *et al* (1979). As it is expected, our calculated cross-sections without Coulomb deflection are slightly higher in the low energy range then those inlcuding the Coulomb deflection and the increase in binding. The peak cross-section of the present calculations ($9{\cdot}46 \times 10^{-20}$ cm$^2$ at about 7 MeV) closely corresponds to the experimental peak cross-section ($9{\cdot}5 \times 10^{-20}$ cm$^2$ at 6·5 MeV) of Sera *et al* (1980) as compared to the scaled peak ($4{\cdot}40 \times 10^{-19}$ cm$^2$ at 7 MeV) of Johnson *et al.* The present calculations including the increase in binding only identically corresponds to

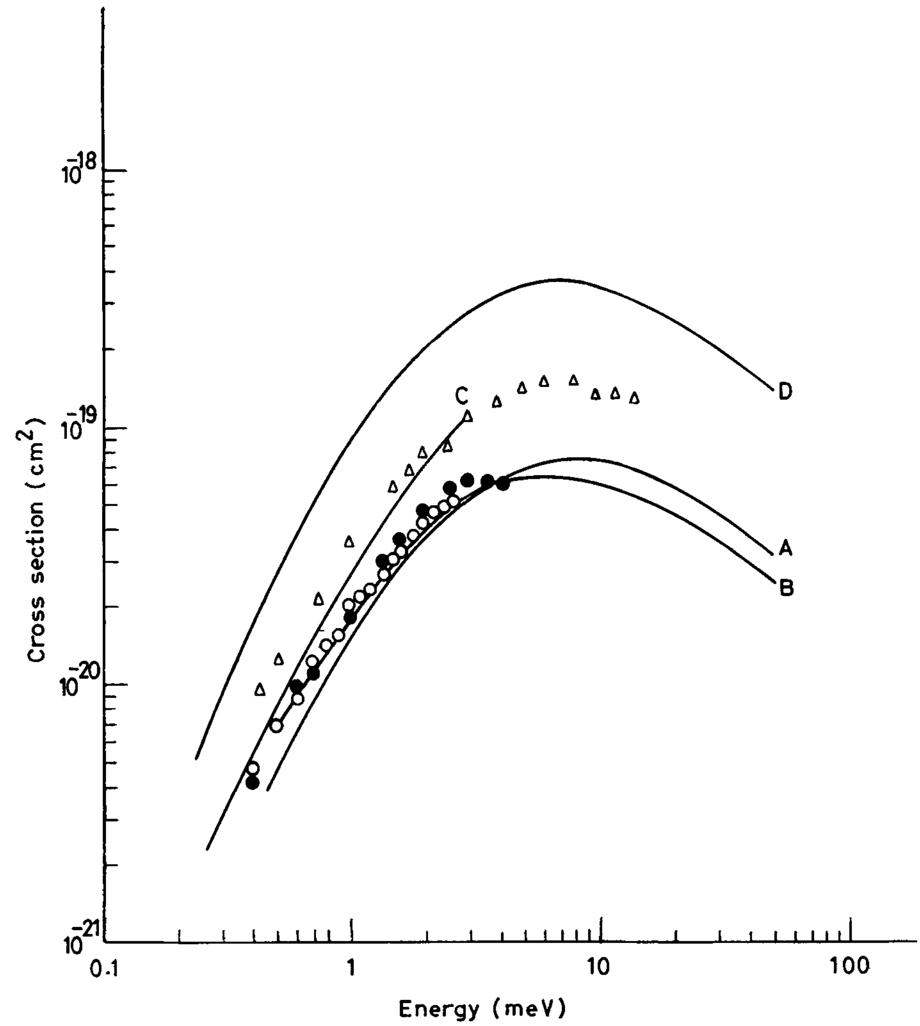


**Figure 2.** Proton impact *M*-shell ionization cross-section of Pb; (A) and (B): Same as in figure 1; (C) ECPSSR calculation of Mehta *et al* (1982); (D) Scaled PWBA results of Johnson *et al* (1979); ● and ○ Same as figure 1; △ Experimental (Busch *et al* 1973).

the experimental peak position and is within a factor of 1·5 from the experimental observation.

Results for proton incident on Pb and Bi are shown in figures 2 and 3, respectively. The present calculations including both corrections for Pb are always in better agreement with the experimental observations of Faria *et al* and Mehta *et al* than the ECPSSR calculations (except in a narrow energy range 0·5 to 0·7 MeV) and the scaled PWBA results. However, our cross-sections understimate the experiment of Busch *et al* (1973) utmost by a factor of 2·5. The peak value of our cross-section ($6{\cdot}48 \times 10^{-20}\,\mathrm{cm}^2$ at 6 MeV) is slightly closer to the experimental value ($1{\cdot}45 \times 10^{-19}\,\mathrm{cm}^2$ at 6 MeV) of Busch *et al* as compared to the peak ($3{\cdot}6 \times 10^{-19}\,\mathrm{cm}^2$ at 6 MeV) of scaled Born calculations. In case of Bi, the present calculations are in better agreement with the experimental results than those of ECPSSR and

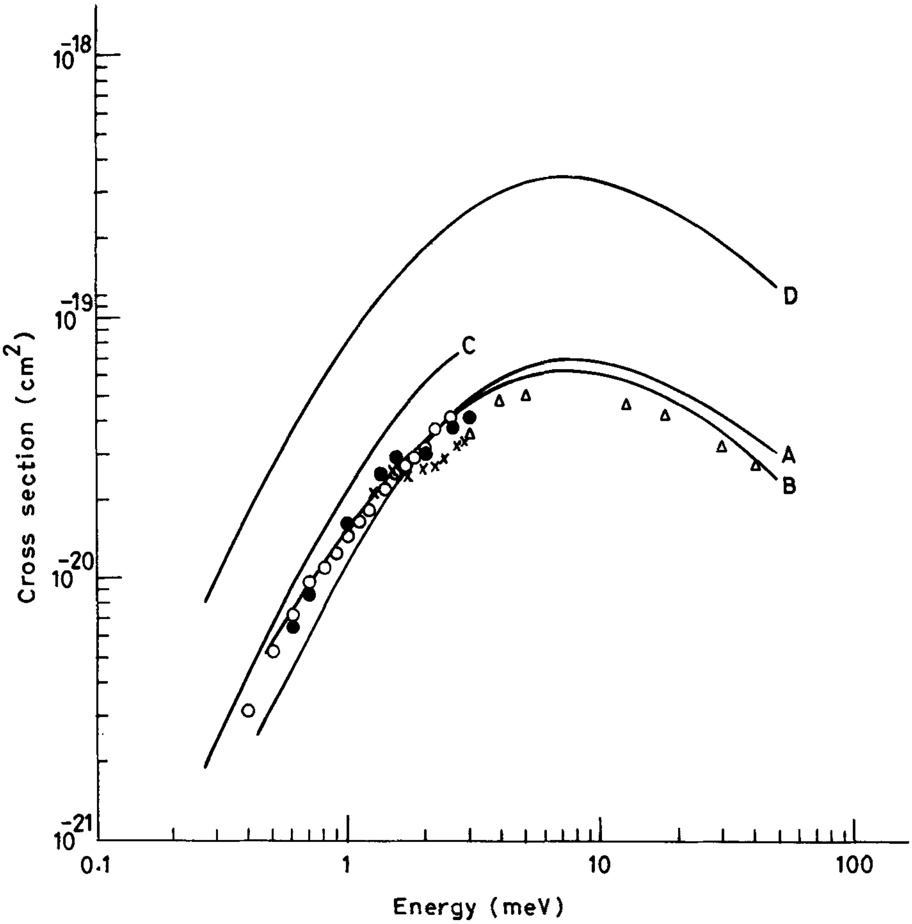


**Figure 3.** Proton impact $M$-shell ionization cross-sections of Bi; (A), (B), (C) and (D): Same as in figure 2; ●, ○ and △ Same as in figure 1; × Experiment (Ishii *et al* 1975).

scaled PWBA throughout the energy range investigated. The peak cross-section of the present calculations ($7{\cdot}0 \times 10^{-20}\,cm^2$ at 7·5 MeV) is closer to the experimental value ($5{\cdot}5 \times 10^{-20}\,cm^2$ at 7 MeV) of Sera *et al* as compared to the scaled PWBA peak cross-sections ($3{\cdot}4 \times 10^{-19}\,cm^2$ at 7·5 MeV). The present calculations without including the Coulomb deflection in the two cases show similar behaviour as in case of Au.

$M$-shell ionization cross-sections for Au and Bi due to impact of $\alpha$-particle along with other theoretical and experimental results are presented in figures 4 and 5, respectively. The present calculations (including Coulomb deflection and increase in binding) underestimate the experimental observations by the largest factor 2·4 below 1·5 MeV and overestimate by the largest factor of 2 above 4 MeV. In the energy range 1·5 to 4 MeV, our cross-sections are in good agreement with experiments. Our calculated cross-sections are in much better agreement with the experimental observations than the scaled PWBA results. As the experimental results are available only up to 5 MeV, it is not possible to estimate the peak cross-sections and to make comparisons with the theoretical ones. The present calculations including only the increase in binding show identical behaviour as in case of proton impact.

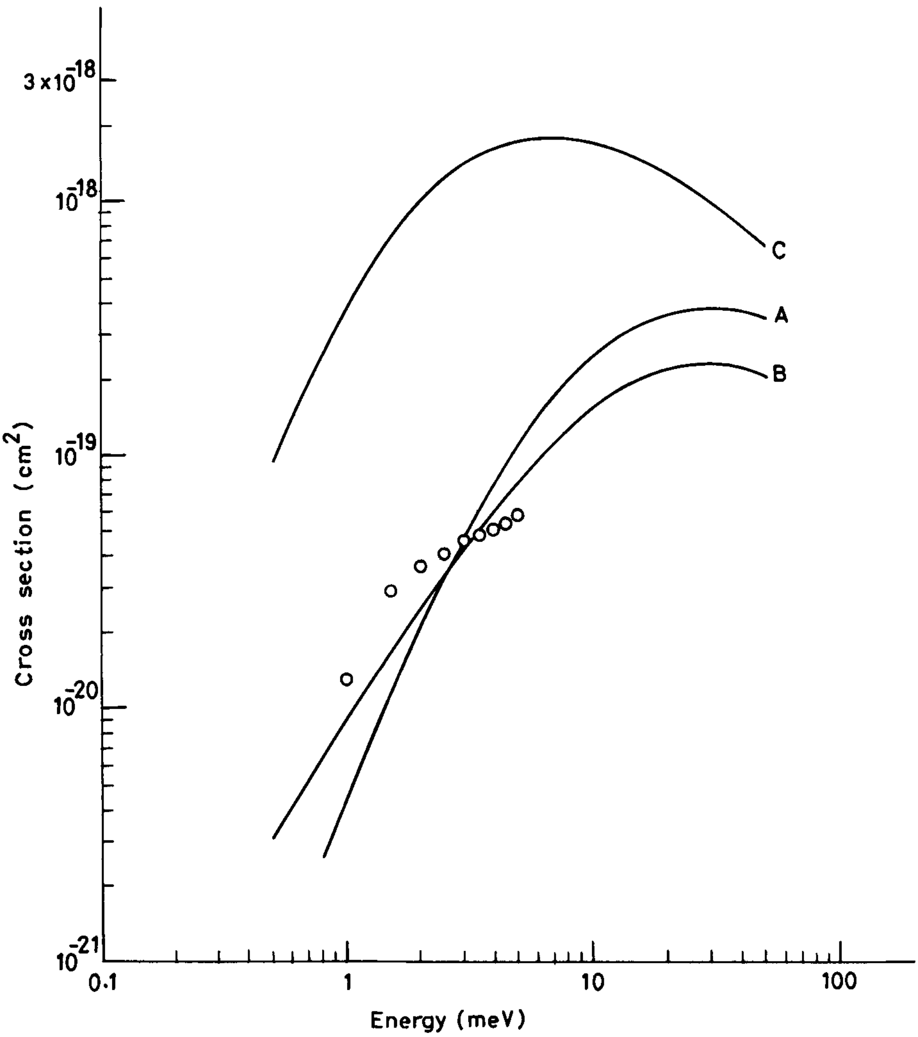


**Figure 4.** α-particle impact $M$-shell ionization cross-sections of Au; (A) and (B): Same as in figure 1; (C) Scaled Born calculation of Johnson *et al* (1979); ○ Experimental (Thornton *et al* 1974).

From figures 1–5, we observe in general (except Au) that the present calculations underestimate the cross-sections in low energy region. This may be attributed to the non-inclusion of the effect of relativistic nature of $M$-shell electron. The charge transfer process may also be supposed to take place at low energy, but Mehta *et al* (1982) have shown that a little contribution comes from this process. The ECPSSR calculations incorporating all the secondary processes overestimate the recent experimental data of Mehta *et al* (1982) and Faria *et al* (1983) throughout the energy range. No explanation has been given for the overestimation of ECPSSR results. The theoretical cross-sections of Chen *et al* (1983), in case of proton impact ionization of Au, are in very good agreement with recent experiments, but their results are limited to 1 MeV only. So, it is difficult to draw any definite conclusion about the agreement of their cross-sections in high energy range. Our calculated cross-sections agree well

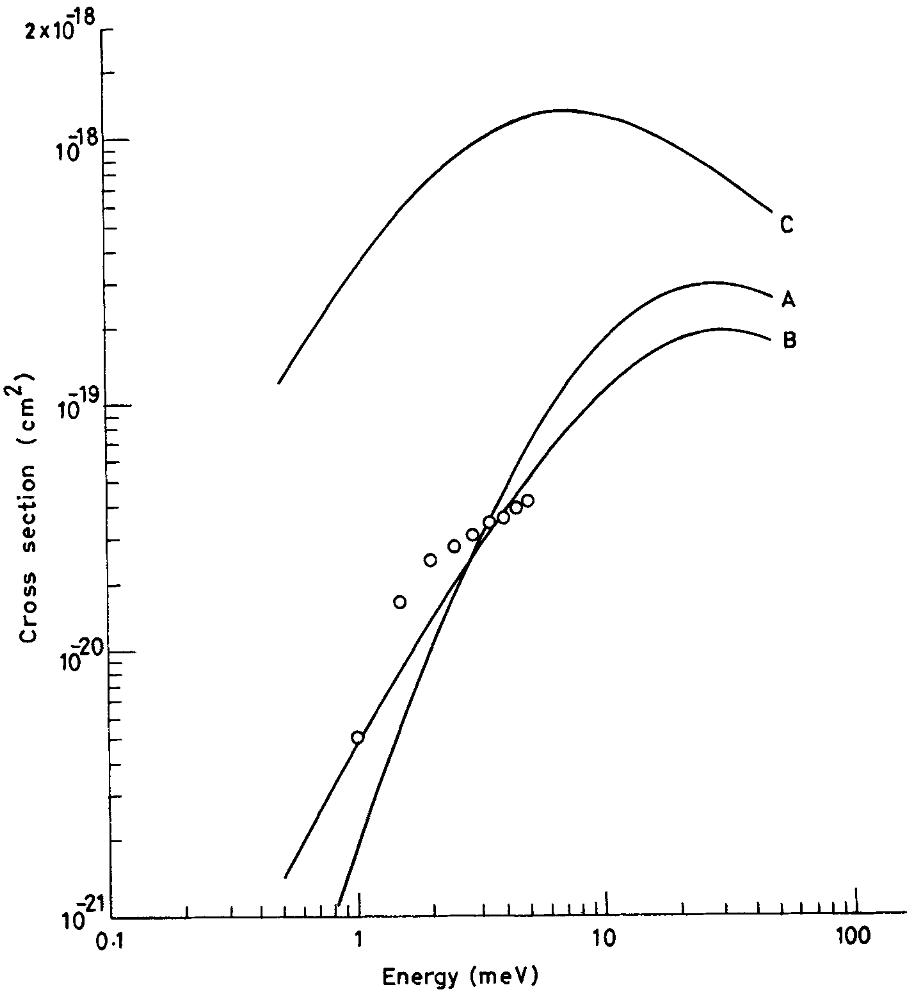


**Figure 5.** α-particle impact $M$-shell ionization cross-sections of Bi; (A), (B) and (C): Same as in figure 4; ○ Same as in figure 4.

with the recent experimental observations in high energy region where no other theoretical calculation has been reported.

In case of α-particle impact, comparatively large discrepancy has been observed in low energy region (below 1·5 MeV). In addition to the non-inclusion of the relativistic contribution, the discrepancy may partly be attributed to the choice of the fluorescence yield. It has been reported that the probability of the multiple vacancy production is large in case of α-particle impact in low energy region (Kauffman *et al* 1973; Richard *et al* 1973). The $\bar{\omega}$ values have been shown to be larger for multiple vacancy than for single vacancy production (see Larkins 1971; Bhalla and Hein 1973). Improved agreement of our cross-sections may be expected by the use of the fluorescence yields including contributions from multiple vacancy production, it available in literature.

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