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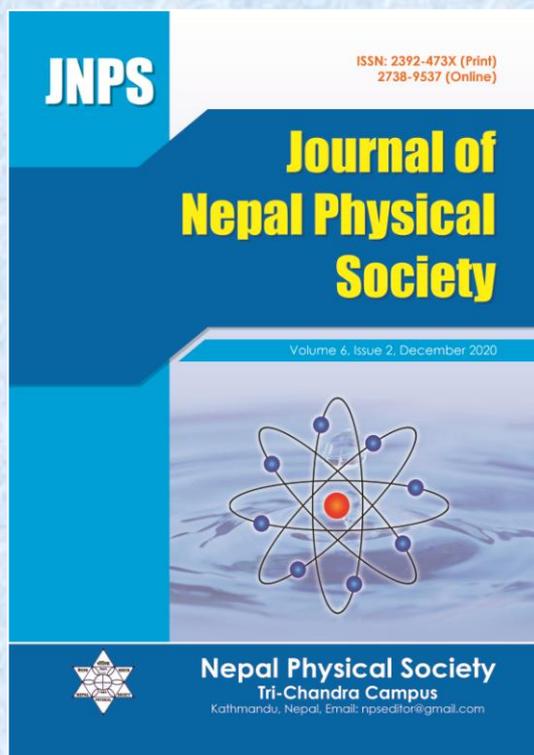
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He²⁺ Impact Single Ionization Cross Sections of Fe Atom

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ABSTRACT

Binary encounter approximation has been used for theoretical calculations of alpha particle (He²⁺) impact single ionization cross sections of iron atom at ground state in the energy range of 35 to 360 keV/amu. The cross sections for energy transfer given by Vriens' and quantum mechanical Hartree-Fock velocity distributions for target electron have been used in the calculation. The contributions in total single ionization cross sections from 4s and 3d subshells are observed to be higher than from 3p, and the contributions from 4s decreases with increase of impact energy whereas the contribution from 3d increases. The total single ionization cross sections decrease gradually with the increase of impact energy similar to experimental results which implies that our results are in satisfactory agreement with the experimental data in the given energy range.

Keywords: Alpha particle impact, Binary encounter approximation, Hartree-Fock velocity distribution, Single ionization cross section (SICS)

1. INTRODUCTION

Single and multiple ionizations of atoms and molecules by ionizing particles like electrons and ions is one of the fundamental processes in atomic physics. Continuous data of ionization cross sections of respective processes have great importance in different fields of science such as modeling of fusion reactor, radiation damage in biological matter (including cancer treatment), upper atmosphere of Titan, plasma processes in comet, planetary atmospheres and biomedical applications [1-5]. Collision with heavy particles like H⁺ and He²⁺ with target atoms may results pure ionization, excitation, excitation-auto ionization, electron capture, charge transfer and transfer ionization. Monte Carlo simulations of track structure are applied in micro-and nanodosimetry to calculate the radiation transport index in the field of medical science. The use of a well validated set of ionization cross section data in such a simulation code ensures accurate calculation of transport parameters. A projectile particle like proton (H⁺) and helium deposit a large amount of their energy in a volume of a few micrometers or even

nanometers and cause extensive damage to the microscope structure of matter and results cell death in the DNA [6]. Charge exchange reactions in various types of ion-atom collisions are of considerable interest due to their applications in different branches of physics like controlled thermonuclear fusion development, astrophysics and in the study of solar corona [7]. The charge exchange processes contribute to the production of negatively charged ions which play an important role in accelerator technology, particularly in the design of tandem accelerator [8]. A large number of elements both in neutral and ionic forms exist in upper atmosphere; the electron capture processes are particularly relevant and important in particle-atom collisions. The emission spectrum of solar chromospheres contains the spectral line of wavelength $\lambda = 4686\text{\AA}$ ⁰ whose origin has been attributed to the presence of ionized helium formed due to the process of electron capture by fast alpha particles (He²⁺).

Description of ionization process with high precision is not possible without considering probabilities of other concurrent process such as

elastic scattering, target excitation and electron capture to the projectile simultaneously in low to intermediate collision energies. It is not possible to describe one process accurately without treating all on equal footing. Electron and heavy charged particles (H⁺, He²⁺) impact direct single and double ionization cross sections for different atoms and ions have been investigated theoretically by many workers. Various quantum mechanical approximations have been used by a number of workers to calculate single ionization cross sections (SICS) for light atoms. Because of the mathematical complexities such approximations are not suitable for heavy target-atoms. Also the theoretical studies of double electron transfer processes using different quantum mechanical approximations are limited only to lighter targets and fails to account heavy target atoms because of complexities involved in theoretical calculation. Several workers carried out the theoretical investigations on pure ionization, ionization due to charge transfer and electron capture processes using modified Gryzinski's formula [9]. The modified binary encounter approximation (BEA) has been used successfully by many workers to calculate direct single and multiple ionization cross sections of several atoms and ions by impact of electron and heavy charged particles like proton and alpha particle. In the past BEA has been used by many workers [10-14] successfully to calculate charge particles impact single and double ionization cross section of atoms and ions.

2. METHODS AND THEORETICAL DETAILS

According to Thomson(1912) consider a situation of collision where the energy transfer in Coulomb collision between a particle of mass m_1 and charge Z_1e with initial kinetic energy E_1 and a particle of mass m_2 and Z_2e with initial kinetic energy $E_2 = 0$ (rest) In the case of binary encounter theory it is assumed that during the period of interaction between projectile and an orbital electron the other electrons and the nucleus play no role. The Thomson's energy transfer(ε) ionization cross section for electron –electron collision is [15].

$$\frac{dQ(\varepsilon)}{d\varepsilon} = \pi \frac{e^4 N}{E_1} \left[\frac{1}{U} - \frac{1}{E_1} \right] \quad (1)$$

For ionization $U \leq \varepsilon \leq E_1$; where U is ionization potential energy.

Thomas and William (1927) modified the formulation for more general case where $E_2 \neq 0$ (considered symmetrical distribution of velocity of target electrons), $m_1 \gg m_2$ and $Z_1 \neq Z_2$ which is relevant to proton and alpha particle –atom collision. Energy transfer ionization cross section has been given as [15].

$$\frac{dQ(\varepsilon)}{d\varepsilon} = \pi \frac{e^4 Z_1^2 Z_2^2 m_1}{m_2 E_1} \left[\frac{1}{\varepsilon^2} + \frac{4E_2}{3\varepsilon^3} \right] \quad (2)$$

In the binary encounter between the incident ion and the target electron the projectile transfers a part of its energy to the atomic electron so that it is ejected out. Thomas theory has been successfully employed by Roy and Rai [8] to specify the limit of energy transfer and later on improved and extended by many workers leading to modified semiclassical binary encounter approximation.

We carry out theoretical calculations of He²⁺ impact SICS of Fe atom using the modified BEA Theoretical approach used in BEA is based on independent particle model. The model is based on the hypothesis that the probability of ionizations is directly related to the energy deposited by the projectile on the target. The energy deposited is statistically distributed among all atomic electrons and one or more of which eventually auto ionize to the final state. An accurate expression of $\sigma_{\Delta E}$ (cross section for energy transfer ΔE) for H⁺ impact given by Vriens [16] and quantum mechanical Hartree-Fock velocity distribution functions for bound electrons of the target atoms or ions have been used to calculate total SICS of iron.

Following McDowell [17], Catlow and McDowell [18] gave an expression of SICS of an atom by electron and H⁺ impact in terms of dimensionless variables s and t . The variables are related to kinetic energies of incoming and orbiting electrons and defined as $s^2 = v_1^2 / v_0^2$ and $t^2 = v_2^2 / v_0^2$, where v_1 and v_2 are the velocities of incident particle and target orbiting electron in atomic units respectively and v_0 is root mean square velocity of orbital electrons. The ionization potential energy of bound electron u is defined as $u = v_0^2$. Atomic

electrons are taken to have a momentum distribution and can be given by Fourier transformation of the Hartree-Fock density distribution electrons. Following Catlow and McDowell, the expression of total SICS for heavy

charged particle impact having energy of $m_1 s^2 u$ with an orbital electron of a particular shell having energy $t^2 u$ is given by

$$Q_i(s) = n_e Z^2 \int_0^\infty Q_i(s, t) f(t) u^{1/2} dt (\pi a_0^2) \quad (3)$$

where n_e is the number of electrons in the shell under consideration, Z is the charge on the projectile (for proton and electron $Z = 1$ and 2 for alpha particle), $f(t)$ is Hartree-Fock momentum distribution function. In the present calculations,

$Q_i(s, t)$ is calculated using an accurate expressions of differential cross section $\sigma_{\Delta E}$ (cross section for energy transfer ΔE) under three different limits of energy transfer as given by Vriens and used by Kumar *et al.* [19].

$$\sigma_{\Delta E} d(\Delta E) = \begin{cases} Ad(\Delta E) & \Delta E \leq 4su(s-t) \\ Bd(\Delta E) & 4su(s-t) \leq \Delta E \leq 4su(s+t) \\ 0 & \Delta E \geq 4su(s+t) \end{cases} \quad (4)$$

$$\text{where, } A = \frac{4}{s^2 u} \left(\frac{1}{\Delta E} + \frac{4t^2 u}{3(\Delta E)^3} \right)$$

$$\text{and } B = \frac{2}{3t(\Delta E)^3} \left(8s - \frac{[(\Delta E + t^2 u)^{1/2} - tu^{1/2}]}{s^2 u^{3/2}} \right)$$

Integration over differential cross section in the above three cases of energy transfer in equation (4) gives $Q_i(s, t)$ for the impact of unit heavy charged particle in terms of dimensionless variables,

$$\begin{aligned} Q_i(s, t) &= \frac{4}{s^2 u^2} \left[1 + \frac{2t^2}{3} - \frac{1}{4(s^2 - t^2)} \right]; & 1 \leq 4s(s-t) \\ &= \frac{2}{s^2 u^2 t} \left[\frac{1}{4(s+t)} + t + \frac{2}{3} \{ 2s^3 + t^3 - (1+t^2)^{3/2} \} \right]; & 4s(s-t) \leq 1 \leq 4s(s+t) \\ &= 0; & 1 \geq 4s(s+t) \end{aligned} \quad (5)$$

The numerical integration of $Q_i(s, t)$ carried out over Hartree-Fock momentum distribution function $f(t)$ of the bound electron that yields

total ionization cross section $Q_i(s)$ [equation (3)]. The momentum distribution function $f(t)$ is defined as,

$$f(t) = 4\pi^2 u \rho_{nl} (u^{1/2} t) \quad (6)$$

where,

$$\rho_{nl} = \frac{1}{2l+1} \sum_{-l}^{+l} |\psi_{nlm}(x)|^2 \quad (7)$$

and

$$\psi_{nlm}(r) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int \phi_{nlm}(r) e^{ik \cdot r} dr$$
 is the Fourier transform of the one electron orbital.

The complete wave function is given by

$$\phi_{nlm}(r) = N_{nl} R_{nl}(r) Y_{lm}(\Omega) \quad (8)$$

where N_{nl} and $R_{nl}(r)$ are the normalization constant and analytical Hartree-Fock radial function, respectively. The empirical relations for N_{nl} and $R_{nl}(r)$ are

$$N_{nl} = [(2n)!]^{-\frac{1}{2}} (2\xi)^{n+\frac{1}{2}} \quad (9)$$

and

$$R_{nl} = r^{n-1} e^{-\xi r} \quad (10)$$

Here zeta (ξ) is orbital exponent of basis function. The spherical harmonic $Y_{lm}(\Omega)$ have different forms depending upon the value of orbital and magnetic quantum numbers l and m respectively. It is well known that velocity of orbital electrons increases with the decrease in shell number and hence electrons of inner shell are relativistic in nature. Here we have ignored the relativistic nature of orbiting electrons. In the present work, ionization from valence shells and few inner shells have only been considered by using non-relativistic wave functions in the mathematical formulation of BEA. Momentum distribution functions for the bound electrons have been constructed using Hartree-Fock radial functions reported by Clementi and Roetti [20]. For shell radii and binding energies of electrons, quantum mechanical value of radial distance of maximum probability given by Desclaux [21] and quantum mechanical value of orbital energies given by Clementi and Roetti have, respectively, been used in the calculations.

Computational calculation of equation (3) finally gives results of SICS for orbitals 4s, 3d and 3p

under different selective constants of respective subshells. The expression of $Q_i(s,t)$ and $f(t)$ are taken from equation (4) and (6) respectively. The momentum distribution function $f(t)$ has been constructed from equations (7-10) for particular orbital electron of the target atom as discussed above. Integration over differential cross section $\sigma_{\Delta E}$ (for energy transfer of ΔE) gives $Q_i(s,t)$ that represents ionization cross section due to a projectile of unit charge for a particular incident energy and particular orbital velocity of bound electron. In our calculations we have considered contributions only from 4s, 3d and 3p subshells as inner shells have negligible effect.

3. RESULTS AND DISCUSSION

The calculated results of He^{2+} impact total SICS of Fe and contribution from individual subshells at different impact energies along with the experimental data have been shown in Table 1 and plotted in Fig. 1.

Table 1: Calculated values of He^{2+} impact SICS of Fe and comparison with experiments

Energy (keV)	Contribution from			Total SICS ($\times 10^{-16} \text{ cm}^2$)	
	4s	3d	3p	Theoretical	Experimental[22]
35	10.7	3.78	0.15	14.63	21 \pm 0.8
40	9.75	4.03	0.18	13.96	23.1 \pm 0.1
47	8.6	4.33	0.21	13.14	22.5 \pm 0.8
54	7.8	4.63	0.24	12.67	22.1 \pm 0.9
62	7.1	4.88	0.27	12.25	20.3 \pm 0.9

75	6.1	5.21	0.30	11.61	18.6±0.9
88	5.5	5.45	0.34	11.29	16.8±0.8
105	4.8	5.67	0.48	10.85	15.1±0.6
125	4.2	5.81	0.41	10.42	13.4±0.5
150	3.6	5.89	0.43	9.92	12.3±0.5
180	3.0	5.86	0.45	9.31	11.3±0.5
213	2.6	5.77	0.46	8.83	9.5±0.4
250	2.2	5.6	0.45	8.25	8.7±0.4
300	1.8	5.34	0.43	7.63	7.7±0.3
360	1.56	5.03	0.4	6.99	6.7±0.3

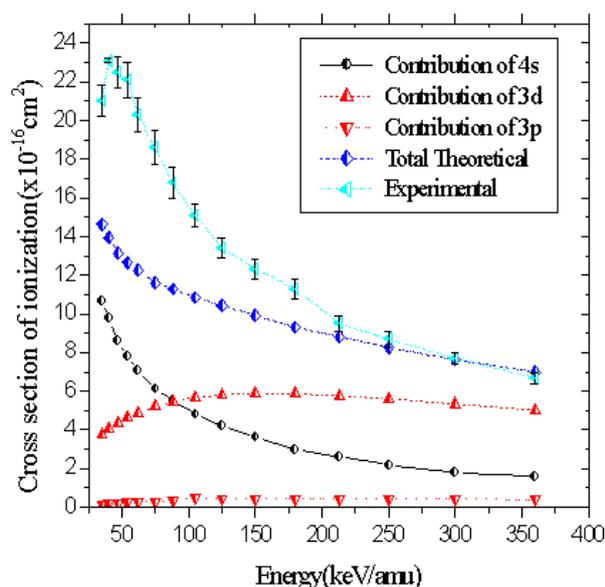


Fig. 1: He²⁺ impact SICS of Fe atom.

The total theoretically calculated SICS for energy range 35 to 360 keV/amu has been compared to the corresponding experimental data (Patton et al. [22]). The contribution of 4s shell is high in threshold range and decreases with increase of impact energy. The contribution from 4s decreases with increase of impact energy whereas the contribution from 3d increases. Result of calculated total SICS decreases gradually with the increase of impact energy. The trend of variation is similar to the experiment as shown in Fig. 1. At the lowest energy of 35 keV/amu the magnitude of theoretically calculated cross section is $14.63 \times 10^{-16} \text{ cm}^2$ while at highest energy of 360 keV/amu it becomes $6.9 \times 10^{-16} \text{ cm}^2$. At impact energy 300 keV/amu and 360 keV/amu the theoretically calculated and experimentally observed values are $7.63 \times 10^{-16} \text{ cm}^2$, $6.99 \times 10^{-16} \text{ cm}^2$ and $7.7 \times 10^{-16} \text{ cm}^2$, $6.7 \times 10^{-16} \text{ cm}^2$ respectively having ratio factor 1.009

and 1.04 respectively. This reveals that results are identical to the experimentally observed values. From the Fig. 1, in general, the experimentally observed values of He²⁺ impact SICS overestimate their corresponding theoretically calculated results. Theoretically calculated results are in close agreement qualitatively and qualitatively throughout the energy range investigated. The theoretically calculated results come closer to the corresponding experimentally observed values with the increase of impact energy. For all values of impact energies ratio factor are within 2. About 66% of results have ratio factors less than 1.5%, 40% have ratio factor less than 1.25 and 20% have less than 1.05. In the intermediate and high energy region theoretical results are very close to experimentally observed values. In the theoretically calculated results contribution of subshells 4s and 3d to the total SICS varies from 76% to 22% and 27% to 72%. As impact energy increases the individual percentage contribution of 4s decreases whereas contribution of 3d gradually increases. Ionization of subshells depends on the electronic energy states. Orbital electrons take part in the process of pure ionization for those that have relatively high energy. Energy of 4s and 3d fluctuates that depend upon the 3d state. The 4s has higher energy when 3d subshell has electrons. Here Fe has 3d⁶ state this is why 4s loses electron first during the interaction with projectile ion. As impact energy increases probability of removal of electron from 3d increases which we observed in theoretical calculations of SICS of Fe. All the theoretically calculated values of SICS fall in valid range having ratio factor within 2 and majority of them are in close agreement with experimentally observed data. The variation of error associated with theoretically calculated results with corresponding experimentally observed values has been shown in Fig. 2. The magnitude of error increases with the

increase of cross section. This reveals that results possess more errors in threshold range where ionization cross sections have high values both in experimentally observed and theoretically calculated values. In the Fig. 2, the linear correlation coefficient (R^2) and standard deviation (SD) of linear fit are 0.9695 and 1.4682. This shows that about 97 % of observed data are in close agreement to the line of best fit and less value of standard deviation certifies that the theoretically calculated results have small uncertainty with respect to experimental data. In low energy range (below 185 keV/amu or above cross section of $10.85 \times 10^{-16} \text{ cm}^2$) the theoretically calculated results are more apart from corresponding experimentally observed values and possess relatively more error compared to intermediate and higher energy region.

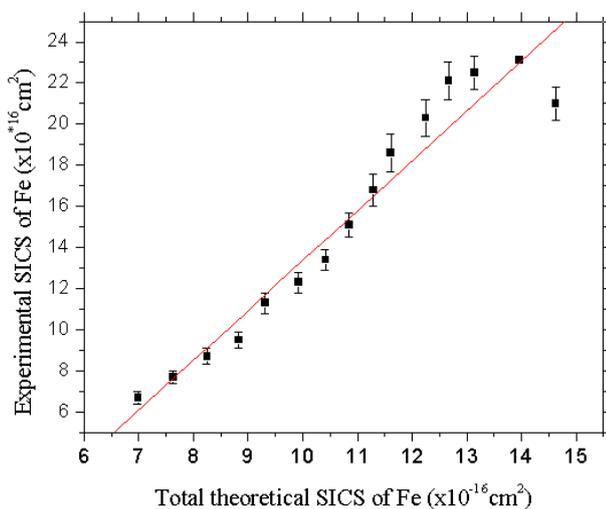


Fig. 2: Linear fit between theoretically calculated and experimentally observed results.

4. CONCLUSIONS

The alpha particle (He^{2+}) impact single ionization cross sections (SICS) of Fe atom at ground state for the range of energies 35 to 360 keV/amu have been theoretically calculated using the binary encounter approximation and Hartree-Fock velocities distribution. It is observed that the He^{2+} impact SICS of Fe are well explained by considering direct ionization of 4s, 3d and 3p subshells. The obtained theoretical results have ratio factor below 2 and nature of variation of total theoretical and experimental curves are nearly same. About 66% of results have ratio factors ≤ 1.5 . Major contribution to the total ionization cross sections are from 4s and 3d for direct single ionization. Contribution of subshells 4s and 3d to the total SICS varies from

76% to 22% and 27% to 72%. Collision interaction at low energy is purely of quantum effect. Various quantum mechanical approximations have been used by a number of workers to calculate single ionization cross sections (SICS) for light atoms. Because of the mathematical complexities such approximations are not suitable for heavy target-atoms. Also the theoretical studies of double electron transfer processes using different quantum mechanical approximations are limited only to lighter targets and fails to account heavy target atoms because of complexities involved in theoretical calculation. The quantum mechanical approaches like Close coupling approximation and Correlation approximation are frequently used for investigation of collision process in the low energy region. In the threshold range there is probability of electron capture, transfer ionization and some complex quantum effects of interaction in between He^{2+} and atomic electrons. The semi classical model does not include all physical insight of ionization in threshold range. Overall the results are in good and satisfactory agreement with the experimental observations for wide range of impact energies.

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