

AN ANALYTICAL EXPRESSION FOR ELECTRON-IMPACT IONIZATION CROSS SECTION

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ABSTRACT

The total cross sections for the ionization of atoms and molecules electron impact have been proposed from close interactions using generalized oscillator strength. The proposed expression is in agreement with the experiments and the other theories.

Keywords: Inelastic scattering, Electron-impact ionization

1. INTRODUCTION

The electron-impact ionization cross sections (EIICs) of atoms and molecules is one of the essential sets of data needed in a wide range of physics and its applications. Separate more detailed information on the electron-impact ionization cross section is also important electron transport for calculating the probability of emitting x-rays subsequent to inner-shell ionization and the accurate description of energy-loss straggling. A number of authors have reported the ionization cross sections for inner-shells (Powell, 1976; Scofield, 1978; Mayol and Salvat, 1990). A work of the systematic of the differential cross section for all shells of atoms and ions have given by Kim (1975; 1983). In a series of publications (Hwang et. al., 1996; Kim et al., 1997; Ali et al., 1997; Kim et al., 1997; Nishimura et al., 1998), a simple analytic formula for the ionization cross section per atomic/molecular orbital are presented using the Binary-Encounter-Bethe (BEB) model (Kim and Rudd, 1994). The electron-impact ionization cross sections of molecules have calculated in a modified first Born approximation by Saksena et. al. (1997). Seltzer (1988) have reported the calculation based on Weizsäcker (1934)- Williams (1935) method for K- and L-shells electron-impact ionization cross sections.

The differential inelastic scattering cross sections of electrons are calculated from a binary-encounter form of Møller cross sections (Møller 1932) to each atomic orbital and a generalized oscillator strength model defined by the electronic configuration and binding energies of the electron shells of the target atoms. This model is similar to that of Sternheimer (1952), Liljequist (1983), Salvat and Fernández-Varea (1992) and Salvat et al. (1985), it is, however, only calculated from close interactions and is included both close and distant interactions. Models based on the free electron gas are unsuitable for describing the electron-(or positron-) impact ionization cross section of inner shells (Mayol and Salvat, 1990). This model is more suitable for the inner-shells ionization. The total electron-impact ionization cross sections of H, He and H₂O have been calculated using this model.

2. THEORY

The differential inelastic scattering cross section (DISCS) can be written by using Weizsacker-Williams method (Weizsäcker, 1934; Williams, 1935) as the sum of DISCSs for distant and close interactions:

$$\frac{d\sigma}{dW} = \frac{d\sigma_d}{dW} + \frac{d\sigma_c}{dW}. \quad (1)$$

The DISCS for distant interactions $d\sigma_d/dW$ is described in terms of the interactions of the equivalent radiation field (virtual photons) with the shell electrons; and the DISCS for close interactions $d\sigma_c/dW$ is described in terms of a interactions between two electrons. The presented study is based on the Weizsäcker-Williams method and the assumptions as follows:

As both distant and close interactions occur between the incident electron and the atomic electron in the same inelastic scattering, the probability of distant interaction equals to the that of close interaction.

Hence DISCS can be obtained by multiplication of DISCS for distant interactions or close interactions with 2:

$$\frac{d\sigma}{dW} = 2 \frac{d\sigma_d}{dW} = 2 \frac{d\sigma_c}{dW}. \quad (2)$$

The DISCS for the close interactions with the i th oscillator is given by Seltzer (1988) as

$$\frac{d\sigma_{ci}}{dW} = \chi f_i P_i \left[\frac{1}{(W + B_i)^2} + \frac{1}{(E - W)^2} + \frac{w}{E^2} - \frac{1 - w}{(W + B_i)(E - W)} + G_i \right], \quad (3)$$

where $w = \left(\frac{E}{E + mc^2} \right)^2$, $\chi = \frac{2\pi e^4}{mc^2 \beta^2}$ (e , mc^2 and $\beta=v/c$ are charge, rest mass energy of

electron and velocity of the incident electron in units of velocity of light, respectively), f_i and B_i are the number of electrons and their binding energy in the i th atomic /molecular orbital, respectively. W is the kinetic energy of the ejected secondary electron. In Eq. (3), the factor

$P_i = \frac{E}{E + B_i + U_i}$ are so-called focusing term, where U_i is the mean kinetic energy of the

electrons in the i th atomic /molecular orbital. The factor

$$G_i = \frac{8U_i}{3\pi} \left[\frac{1}{(W + B_i)^3} + \frac{1}{(E - W)^3} \right] \left[\arctan \sqrt{y} + \frac{\sqrt{y}(y-1)}{(y+1)^2} \right], \quad (4)$$

with $y=W/U_i$, is the result of averaging over an isotropic, hydrogenic distribution of orbital electron velocities (Seltzer 1988).

After an inelastic scattering of the incident electron with the atomic electrons, incident and atomic electrons are indistinguishable; we consider that the incident electron is the most energetic electron and hence the maximum energy loss is $W_m=(E-B_i)/2$ for electrons.

3. RESULTS AND DISCUSSION

The EIICS for i th inner-shell $\sigma_i(E)$ is calculated from

$$\sigma_i(E) = 2 \int_0^{W_m} \frac{d\sigma_{ci}}{dW} dW, \quad (5)$$

as

$$\sigma_i(E) = 2\chi_i^f P_i \left[(E - B_i) \left(\frac{1}{EB_i} + \frac{w}{2E^2} \right) + \frac{1-w}{E+B_i} \ln \left(\frac{B_i}{E} \right) + \int_0^{(E-B_i)/2} G_i dW \right]. \quad (6)$$

The total EIICS $\sigma_{imp}(E)$ can be written as

$$\sigma_{imp}(E) = \sum_{i=1}^M \sigma_i(E) \theta(W - B_i), \quad (7)$$

where M is the number of atomic/molecular orbitals and $\theta(x)$ is the step function ($\theta(x)=0$ if $x<0$ and $\theta(x)=1$ if $x\geq 0$). The total EIICSs obtained using Eq. (7) are compared with the theory (Kim and Rudd 2000), to be referred to as the Binary-Encounter-Bethe (BEB) model (Kim 1994) and with the experimental data (Shah et. al., 1987; Shah et. al., 1988; Montague et. al., 1984; Straub et. al., 1998; Rao et. al., 1995; Duric et. al., 1988; Bolarizadeh et. al., 1985; Schutten et. al., 1966) quoted from Kim and Rudd (2000), in the energy regions $B_v < E \leq 5$ keV for H and $B_v < E \leq 2$ keV for He and H₂O in Figures 1-3, where B_v is the binding energy of weakly bound electrons in the target atom/molecule. The oscillator strengths f_i , the binding energies B_i and the mean kinetic energies U_i of atomic/molecular orbitals for H, He and H₂O are taken from Kim and Rudd (2000). The presented expression agree quite well with BEB model and the experimental data.

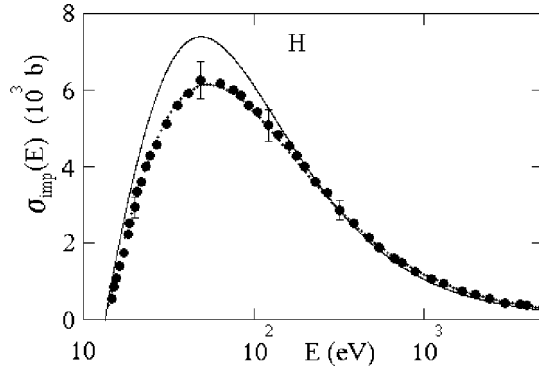


Figure 1: Electron impact ionization cross section $\sigma_{\text{imp}}(E)$ for H as a function of the electron kinetic energy E . The curves are calculations from — : this study, : Kim and Rudd (2000). The points, • are measurements from Shah et. al. (1987).

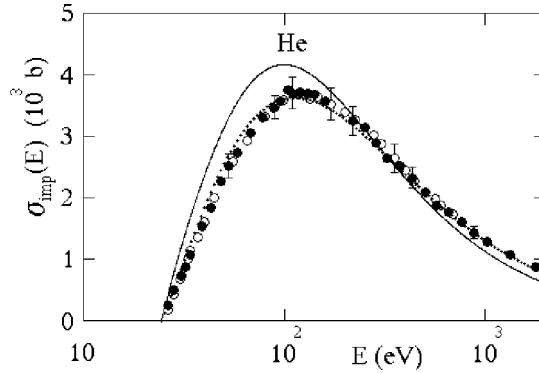


Figure 2: Electron impact ionization cross section $\sigma_{\text{imp}}(E)$ for He as a function of the electron kinetic energy E . The curves are calculations from — : this study, : Kim and Rudd (2000). The points, • : are measurements from Shah et. al. (1988), ○ : Montague et. al. (1984).

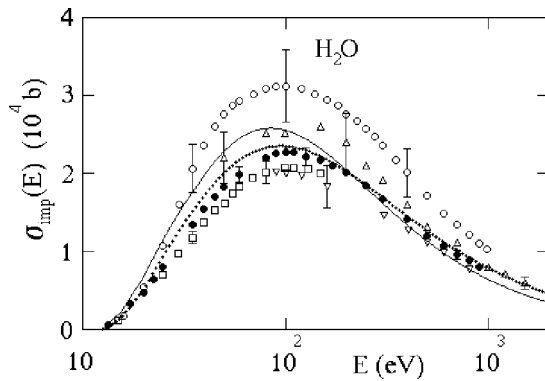


Figure 3: Electron impact ionization cross section $\sigma_{\text{imp}}(E)$ for H_2O as a function of the electron kinetic energy E . The curves are calculations from — : this study, : Kim and Rudd (2000). The points are measurements from • : Straub et. al. (1998), ○ : Rao et. al. (1995), □ : Duric et. al. (1988), △ : Bolarizadeh et. al. (1985), ▽ : Schutten et. al. (1966).

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