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Calculating the Atomic electron impact Ionization Cross Section for some elements

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Abstract

Inner-shell ionization cross section (ICS) by electron impact are of interest not only to the basic collision physics for complex atoms, but also to various practical applications in material science and electron microscopy. Theoretical difficulties in the past were between the threshold and the peak, which occur usually four to five times the threshold energy. Theories based on classical mechanics are somewhat better than on Born cross section, but such theories usually requires adjustable parameters. We used the Gryzinski formalism to calculate atomic electron impact ionization cross sections for the elements (*Fe,Co,Mn,Ti,Zn,& Nb*). Good to satisfactory agreement was found for all atoms with the exception of (*Nb*), where the distance between our cross section and Deutsch-Mark formula become larger at the high values of the overvoltage (U). Moreover, when compared to other to available ionization cross sections for these atoms, calculated using other methods and semiempirical formula, the Gryzinski formalism achieved a level of agreement with experimental data that is as good better than the predictions from the other methods.

حساب المقاطع العرضية للتأين الالكتروني لبعض العناصر

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الخلاصة

المقاطع العرضية لتأين القشرة الداخلية لتصادم الالكترونات هي من الاهمية ليس فقط لمبادئ فيزياء التصادم، لكنها مهمه للعديد من التطبيقات العملية لعلم المواد ومطيافية الالكترون. في الماضي كانت الصعوبات النظرية تبرز ما بين العتبة والقمة، والتي تكون عادة اربعة أو خمسة اضعاف طاقة العتبة. ان النظريات التي تعتمد الميكانيك الكلاسيكي هي نوعاًما أفضل من تلك التي تعتمد المقاطع العرضية لبورن، ولكن مثل هذه النظريات تتطلب استخدام معاملات تعديل. لقد قمنا بتطبيق صيغة كرايزنسكي لحساب المقاطع العرضية للتأين الالكتروني للعناصر (الحديد، الكوبلت، المنغنيز،

التيتانيوم، الزنك، والنبيوم). التوافق كان جيدا بين حساباتنا والقراءات الاخرى لكل الذرات ماعدا النبيوم، حيث ان المسافة تصبح اكبر مابين المقاطع العرضية الخاصة بنا وتلك المحسوبة بصيغة ديتش-مارك عند القيم العالية ل (U) . ان طريقة كرايزنسكي اعطت نتائج جيدة والتي قورنت مع الصيغ النظرية والشبة تجريبية والقراءات العملية الاخرى.

1.Introduction

During the past decade, several powerful theoretical methods to calculate electron-impact ionization cross sections for the atoms have emerged in the literature[1-5]. These methods essentially solve the Schrodinger equation for two electrons with both electrons in the continuum, and are in principle capable of deducing differential ionization cross sections as well as total ionization cross sections. The detailed, sometimes overwhelming, volume of collision data from these theoretical methods requires substantial computational resources, and many of the methods are limited to one-electron model [3].

We anticipate that these fundamental theories will eventually provide collision data for atoms with the study progress in computing power. Until such time, however, there is an acute need for simple, flexible, and reliable theoretical methods to calculate electron-impact total ionization cross sections for the large number of atoms in a wide range of scientific and industrial applications, such as in astrophysics, atmospheric science, x-ray, lasers, magnetic fusion, radiation physics, semiconductor fabrication [3]. For such applications ionization cross sections must be reliable not only at high incident energies, but also at low and intermediate incident energies [6].

In this article theoretical total ionization cross sections, which were calculated using a combination of the Gryzinski models [7,8], for direct ionization cross sections, are compared to available experimental and theoretical data [9,10] on iron, cobalt, manganese, titanium, zinc, niobium. For those atoms several issues must be addressed to obtain reliable total ionization cross sections.

The first issue is the initial state of the target atoms. Because most atoms have metastable terms close to the ground term with the same electronic configuration a substantial number of target atoms may be such metastable terms depending on the way the target atoms are prepared in an experiment. The second issue is that in most experiments is made of the final state of the ions produced. Most atoms will produce ions that also have metastable terms with the same electronic configuration as the ground term of the ion. This

problem solved in a rigorous theory by choosing the appropriate exit channels [3].

The knowledge of the energy distribution of the electrons in the solid i.e. (ionization cross section), the energy variation of the ionization cross sections of the subshell is required to calculate the intensity of x-ray emission in electron beam microanalysis[11]. The calculation of x-ray emission spectra by KeV electrons is generally difficult, mostly because bremsstrahlung emission and inner-shell ionization occur with very small probabilities in comparison with the dominant interaction mechanisms of elastic scattering [12].

2.Theory

The complete theory is given elsewhere [6-8], so in this paper only the essential points will be summarized. An electron with energy (E) ionizes an inner shell with binding energy (E_B), and in the process is emerging with energy (E') and ejecting an electron of energy (ε) from the atom. Conservation of energy requires that:

$$E - E' = E_B + \varepsilon \quad \text{.....(1)}$$

The ionization cross section (ICS) formulated by Gryzinski [7,8] used the classical theory of inelastic collision – the binary encountered approximation- for each orbital (ℓ) to obtain:

$$\sigma_\ell(E) = (\frac{\sigma_0}{E_{B,\ell}^2}) g_\ell(U) \quad \text{.....(2)}$$

Where, $\sigma_\circ = (6.56 * 10^{-14} eV^2 cm^2)$, and $(E_{B,\ell})$ is binding energy of electron in orbital (ℓ) under study.

$$g_\ell(U) = \frac{1}{U}(\frac{U-1}{U+1})\left[1 + \frac{2}{3}(1 - \frac{1}{2U})\ln(2.7 + (U-1)^{1/2})\right] \quad \text{.....(3)}$$

Where g_ℓ is a function changing in amount for each incident energy (E).

It is well known that the ionization cross section typically rises from threshold to a maximum at about $(3E_B)$, and then slowly falls of. Since this behavior is universal it is often convenient for comparison purposes to plot the cross section against the overvoltage (U), the ratio of the electron energy to the binding energy

$$U = \frac{E}{E_B} \quad \text{.....(4)}$$

All the data we have present it are compared with the calculations of Deutsch et al.[9]. They proposed overcoming large-scale quantum chemistry

atomic calculations by using a limited number of parameters or explicit relationship, giving rise to the so called modified additive rule (MAR). The Deutsch-Mark (DM) formalism express the shell ionization cross section (σ_{ion}) as:[5]

$$\sigma_{ion} = g_S \pi (r_S)^2 \xi_S f(U) F(U) \quad \ldots\ldots\ldots\ldots\ldots\ldots (5)$$

Where $(r_S)^2$ is the radius of maximum radial density of the atomic shell; (ξ_S) the number of electrons in the shell; and (g_S) is a weighting factor. The energy dependence of the shell ionization cross section is given by the product of the two functions *f(U)* and *F(U)*. The function *f(U)* is similar (but not identical) to the energy dependence first given by Gryzinski [7,8] and has the form:[9]

$$f(U) = d\left(\frac{1}{U}\right)\left[\frac{(U-1)}{(U+1)}\right]^a \left\{b + c[1-(2U)^{-1}]\ln[2.7+(U-1)^{1/2}]\right\} \quad \ldots(6)$$

Where the parameters *a, b, c* and d have the following values: *a*=1.06, *b*=0.23, *c*=1.00, and *d*=1.1. The function *F(U)* is relativistic correction factor, which is again similar (but not identical) to the one introduced by Gryzinski [7,8] and has the form:[9]

$$F(U) = R(U)\left[1 + \frac{2(U)^{1/4}}{(J)^2}\right] \quad \ldots\ldots..(7)$$

With $J = (m_e c^2)/E_B$, and with m_e being the electron mass. The function R(U) is given by

$$R(U) = (1+2J)/(U+2J) \times [(U+J)/(1+J)]^2 \{[1+U)(U+2J)(1+J)^2]/ [J^2(1+2J)+U(U+2J)(1+J)^2]\}^{3/2} \quad \ldots..(8)$$

3.Results & Discussion

As we mentioned in the theory that the entire theoretical procedures and equations are given in our published research represented in Ref.[6], where we present how to calculate the electron energy. Whereas the mean equation used in calculating the ionization cross section is equ.(2), to be notice.

Since our theoretical model is simple and accuracy of the available experimental ionization cross sections is modest, it is not necessary for us to know the details of the Auger process, such as fluorescence yields and particle cross sections for the numerous channels of Auger decay. It is sufficient for us

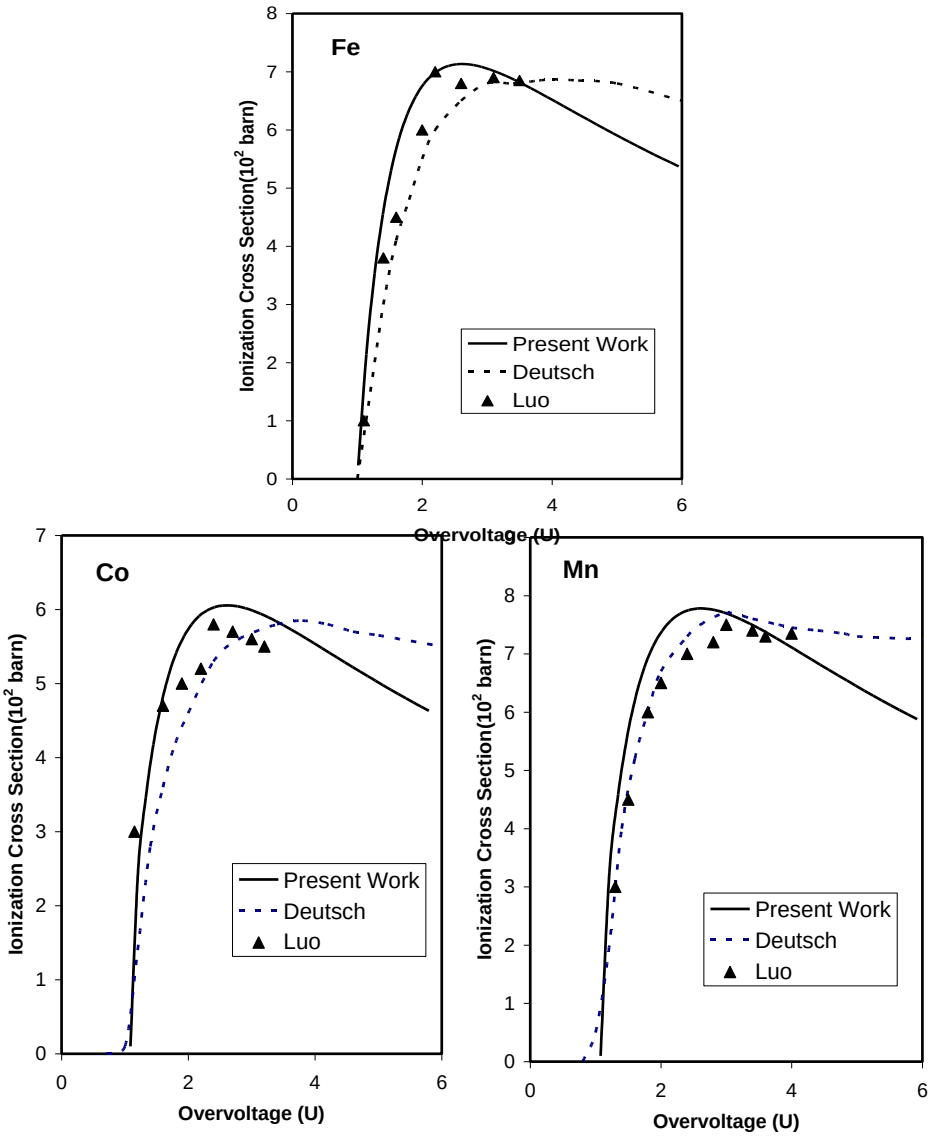
to consider only the energy balance from the list of orbital binding energies in Table(1) [5].

In figures(1,2) we present our result of the (ICS) of (*Fe, Co, Mn, Ti, Zn, Nb*)-atoms interacting with projected electrons at intermediate energies. In this figures we made a comparison with the theoretical data of Deutsch et al.[9] and measurements of Lue et al.[10]. In general the agreement was good for all systems except for (*Nb*), it was satisfactory, where the distance between our results of the (ICS) and those of Deutsch-Mark formula become larger at the high values of (U), if we compare it with the results of other elements under study. Those atoms have metastable terms with the same electronic configuration, ($4s^2$) for all atoms except for (*Nb*)-atom it was (5s), as their ground terms and with different total spin and total orbital angular momentum. The existence of metastable target atoms can often be confirmed in experiments by significant ionization below the correct ionization threshold for the ground term, because metastable terms have lower ionization energies.

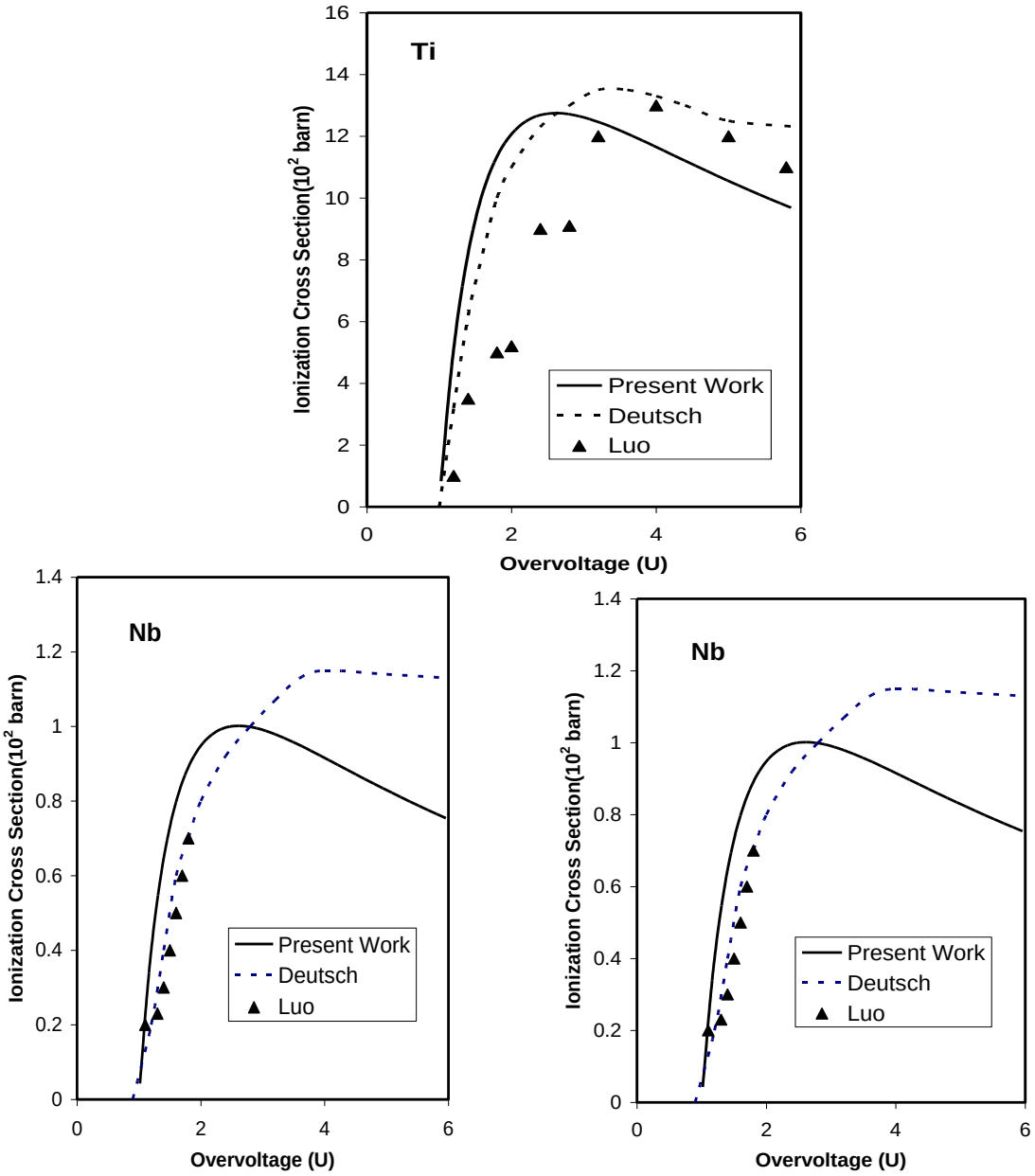
The energy distribution of electrons in the specimen or (ICS) can be modeled either numerical solutions of Boltzmann transport equations or Monte Carlo calculations. Each method has its strengths and weakness. In Boltzmann transport equations has been used a fast and efficient numerical solutions, but are limited in the number of energy levels that can be used. Monte Carlo calculations can be used with arbitrary specimen geometries, but care should be taken that the sampling is done correctly and that simple approximations such as continuous slowing down do not lead to significant error.

Table(1): present the binding energy (E_B) for atoms under study, for the entire range of the incident energy(E) ;Z, the atomic number:[5]

Element	Z	$E_B(eV)$	$U = \frac{E}{E_B}$	$\sigma_{ion}(10^2 barn)$
Fe	26	7.897	2.659	7.131
Co	27	8.279	2.657	6.055
Mn	25	7.434	2.555	7.777
Ti	22	6.82	2.639	12.749
Zn	30	9.393	2.661	3.696
Nb	41	6.882	2.615	1.001



Figure(1):Comparison of ionization cross section for (Fe, Co, Mn); U, overvoltage; solid curve, the presnt work; dashed curve, data theory of Deutsch et al.[9]; triangles, experiment data by Lue et al.[10].



Figure(2):Comparison of ionization cross section for (Ti, Zn, Nb); U, overvoltage; solid curve, the presnt work; dashed curve, data theory of Deutsch et al.[9]; triangles, experiment data by Lue et al.[10].

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