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Measurement of scandium and vanadium K-shell ionization cross sections by electron impact

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Abstract. Electron impact Sc and V K-shell ionization cross sections have been measured for the first time in the incident energy region from near threshold to 45 keV. Thin targets with thick substrates are used in the experiments. The influence of the substrate on measured data has been corrected by a method based upon an electron transport calculation. For Sc and V elements, the experimental data are compared with some empirical formulae and theoretical results. It is found that the experimental data for Sc and V and most of the other elements measured before (i.e. Ti, Cr, Mn, Fe, Co, Ni, Cu, Zn, Nb and Mo) with the same method as presented in this paper, can be reasonably described by both Luo's theoretical results and Casnati's empirical formula.

1. Introduction

Cross sections for the removal of atomic inner-shell electrons by electron impact are needed in many branches of physics such as plasma physics, astrophysics, electron–matter interaction and quantitative microanalysis by electron probe [1]. In addition, these data are of basic importance for better understanding the electron–atom interaction.

In recent years, the study of ionization cross sections of atomic inner shells by electron impact has been of growing interest experimentally [2–11] and theoretically [3, 12, 13]. Many calculations of the cross sections have been made in classical and quantum mechanics. For example, Gryzinski [14, 15] developed a most successful classical model for atomic excitation and ionization. It has been widely used largely because of its simplicity, analytical convenience and supposed applicability to all shells, and it can well describe a wide range of experimental data except close to threshold (overvoltage $U_k = E_\mathrm{i}/E_k < 4$, E_i is the incident electron energy, E_k threshold energy). The most recent quantum mechanical calculations have been presented by Khare and Wadehra [12] and Luo [13]. Khare and Wadehra employed a plane-wave Born approximation (PWBA) with exchange, Coulomb and relativistic corrections and included the transverse interaction of virtual photons with atoms as well, and good agreement with experimental data is obtained for $1 < U_k < 10^4$. Luo performed an extensive series of calculations using first-order perturbation theory and Hartree–Slater wavefunctions for K, L (L_1 and L_2) and M (M_1, M_{23} and M_{45}) shell ionization cross sections for incident electron energies ranging from near threshold to 100 keV. Exchange and correlation energy effects were included in the calculation. More detailed reviews of theoretical calculations of inner-shell

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ionization cross sections were given in [1,12] and [16]. On the other hand, due to the difficulty of deriving simple analytical formulae from an accurate theoretical treatment, a number of semi-empirical and empirical formulae have been proposed [1, 16]. These analytical expressions can be useful in algorithms developed for microanalysis. Most recently, Hombourger [16] proposed an empirical formula, based upon the analysis of expanded databases, to describe the K-shell ionization cross sections over a wide range of atomic numbers (i.e. $6 \leqslant Z \leqslant 79$) and overvoltages U (i.e. $1 \leqslant U_k \leqslant 10^4$).

According to the compilations of Long *et al* [17] and Joy [18,19], it can be found that until ten years ago experimental K-shell ionization cross sections by electron impact were scarce in the low-energy region (i.e. $U_k \leqslant 4$) and discrepancies among these data from different measurements for some atoms were apparent. In recent years, major progress in measurement in the low energy region has been made by Luo *et al* [5–11]. Thin targets with thick substrates were utilized in their experiments, and effects of the reflected electrons from thick substrates were corrected based upon an electron transport calculation [6, 20]. Their method has the advantage of circumventing the difficulties of preparing self-supporting thin targets and has been applied to measure K-shell ionization cross sections for some atoms.

In this paper, we employ the same method to measure the K-shell ionization cross section of scandium and vanadium, for which experimental data do not exist to our knowledge. Comparison of the experimental data of scandium and vanadium and of other elements measured before with the same method with some empirical formulae and theoretical results is presented.

2. Experiment

The experimental details have been given elsewhere [6, 8]; here only a brief description of the experiment is presented. The experimental setup is identical to the one we used earlier [8].

The electron beam current from near the threshold to 45 keV was provided by an electron gun and adjusted in accordance with the x-ray counting rate; the energy of the incident electron beam was determined by the end-point of the obtained bremsstrahlung spectrum. With this method, the incident electron energy can be measured within an uncertainty of 0.1 keV. All charges of the electron beam were collected by a deep Faraday cup and were led to a digital current integrator. The current integrator has been calibrated by a standard current source before measurement and its uncertainty was found to be less than 0.3%.

The targets used in our experiments were prepared by evaporating Sc and V elements onto an aluminum substrate by using vacuum coating technology; their thickness was monitored and measured by a quartz oscillator. The uncertainty of the target thickness should be less than 10%. The purity of the targets was better than 99.9% and the homogeneity of the targets was probed by recording beam-induced x-rays from different spots of the targets. The target thickness is listed in table 1. The thickness of the substrate was much larger than the range of the electron with an energy of 45 keV. The targets were placed at 45° with respect to the beam direction, and the characteristic x-rays emitted from the target atoms were detected by an Si(Li) detector positioned at 90° to the electron beam. The detector FWHM (full width at half maximum) was 180 eV for ^{55}Mn K_α x-rays. The K_α and K_β peaks of Sc and V elements in the experimental x-ray spectra can be clearly distinguished from the continuous bremsstrahlung background and other peaks from L, M shells of Sc and V and from the characteristic x-rays of the Al substrate. The detection efficiency calibration of this system was performed [11, 21] with standard radioactive sources, i.e. ^{241}Am, ^{137}Cs, ^{55}Fe and ^{54}Mn, provided by the China Institute of Atomic Energy. The uncertainty of the calibrated efficiency was believed to be less than 5%.

Table 1. Relevant parameters for the calculations of the Sc and V K-shell ionization cross sections.

	Z	A	ω_k	E_k (keV)	I_β/I_α	ρd (μg cm^{-2})
Sc	21	44.96	0.190	4.490	0.131	9.9
V	23	50.94	0.250	5.466	0.134	26.1

The repeatability of measured cross section data was also checked, and repeatedly measured cross sections were found to be consistent within an uncertainty of 1.5%.

3. Results and analysis

As mentioned in section 1, the measured cross sections should be corrected due to the existence of the thick substrate. The correction method used here has been described in detail in [5, 6]. Here the final formula for the K-shell ionization cross section Q_k is given as follows:

$$Q_k(E) = \left(\frac{4\pi}{\eta\Omega}\right)\left(\frac{N_x(E)\mathrm{A}\cos\theta}{N_\mathrm{A}N_\mathrm{e}\omega_k\rho\,\mathrm{d}}\right)\left(1+\frac{I_\beta}{I_\alpha}\right) - \cos\theta\int_{E_k}^{E}\Phi_\mathrm{ref}(E')Q_k(E')\,\mathrm{d}E' \qquad (1)$$

where ω_k is the K-shell fluorescence yield, $N_x(E)$ denotes the K_α x-ray counts, N_e means the number of incident electrons, N_A and A are the Avogadro constant and atomic weight, respectively, ρ is the target density, d is the target thickness, I_α and I_β refer to K_α and K_β x-ray intensities, respectively, and θ is the angle between the incident beam direction and vertical direction of target plane. $\eta\Omega/4\pi$ is the total detection efficiency for K_α x-rays. Φ_ref, the reflection energy spectrum, is calculated by using the bipartition model of electron transport [20]. After performing iterations in equation (1), the corrected K-shell ionization cross sections can be obtained. In general, compared to the uncorrected cross sections, the corrected ones will decrease by 10–30%. The relevant parameters used for calculation of Q_k were taken from [22] and are listed in table 1. Recently, a set of fluorescence yields has been reviewed by Hubbell *et al* [23], but in the present calculations for K-shell ionization cross sections of Sc and V the fluorescence yields given by Bambynek *et al* [22] in their 1972 review article are used, in order that in the following paragraph all experimental data measured before with the same method based upon the same fluorescence yields of Bambynek *et al* [22] can be analysed together on a consistent basis (in fact differences between the two sets of fluorescence yields for the elements of interest here are less than 3%). The present experimental results for Sc and V elements are plotted in figures 1 and 2 and also listed in table 2 (E_i refers to incident electron energy; the numbers in parentheses refer to total errors). Errors mainly arise from net peak counts (1–5%), detection efficiency (5%), fluorescence yield (6%), target thickness (10%) and inhomogeneity of the target (4%). Therefore, the total uncertainty is estimated to be less than 15%. In addition, the contribution of the continuous bremsstrahlung spectrum to the measurement was estimated and found to be less than 1% [21].

Powell has made a comparison [24] of several widely used empirical formulae (i.e. of Casnati *et al* [25], Jakoby *et al* [26] and Deutsch *et al* [27]) and of some theoretical results (i.e. of Gryzinski [14, 15], Khare and Wadehra [12] and Luo [13]) with experimental data of K-shell ionization cross sections for C, N, O, Ne, Al, Ar, Fe, Ni, Cu, Mo and Ag. It was found that the empirical formula of Casnati *et al* was superior to the equation of Gryzinski and to the empirical formulae of Jakoby *et al* and Deutsch *et al* and that the theoretical results of Khare and Wadehra [12] were generally larger than the experimental data, and the theoretical results of Luo [13] can agree reasonably with the measured data. Recently, Hombourger [16] also observed that the empirical formula of Casnati *et al* is superior to the others. In addition, in the

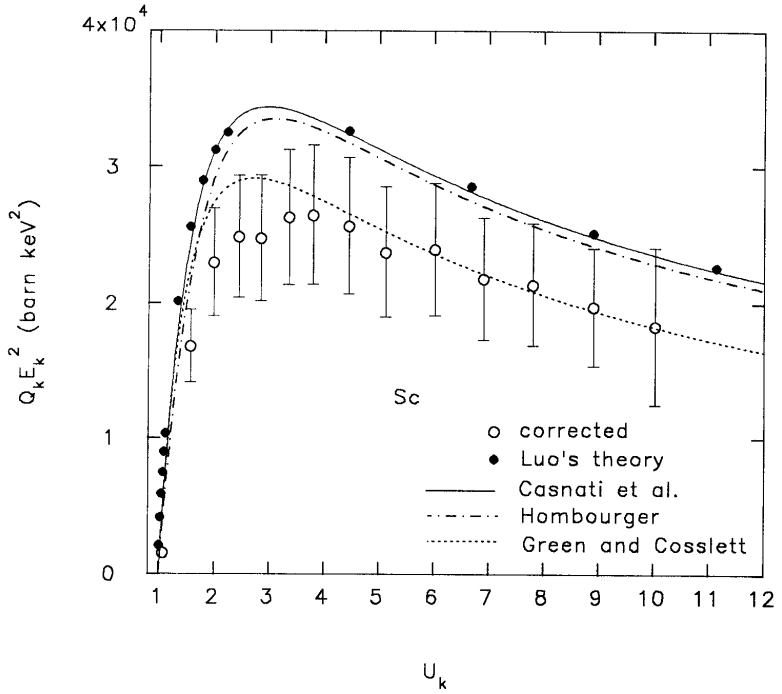

Figure 1. Plots of $Q_k E_k^2$ versus U_k for Sc. The solid and dash–dotted curves represent the results of the empirical formulae of Casnati *et al* and Hombourger, respectively. The dotted line exhibits the results of the semi-empirical formula of Green and Cosslett. Luo's theoretical results are denoted by solid circles. The corrected experimental data are shown by hollow circles.

Table 2. Corrected K-shell cross sections Q_k (barn) and errors for Sc and V elements in the present experiment.

Element	E_i (keV)	Q_k (barn)	Element	E_i (keV)	Q_k (barn)
Sc	4.8	76(±14)	V	5.9	34(±5)
	7.1	832(±135)		7.9	455(±59)
	8.9	1140(±196)		9.9	764(±104)
	11.0	1233(±222)		11.7	905(±128)
	12.8	1228(±228)		14.0	991(±144)
	15.1	1304(±244)		16.2	1083(±160)
	17.1	1312(±253)		20.0	1105(±169)
	20.0	1272(±247)		24.0	1044(±165)
	23.0	1177(±237)		28.0	988(±161)
	27.0	1188(±241)		32.0	977(±159)
	31.0	1081(±224)		36.1	850(±147)
	35.1	1059(±225)		39.9	817(±151)
	40.0	977(±217)		45.0	794(±162)
	45.0	907(±289)			

paper of Hombourger [16], we can see that the proposed empirical formula was in part based upon the measured cross sections of Luo *et al* [5–9] and its prediction for K-shell ionization cross section was similar to that of Casnati *et al*. Therefore, in the present paper we choose the theoretical results of Luo [13] and the empirical formula of Casnati *et al* [25] to compare with

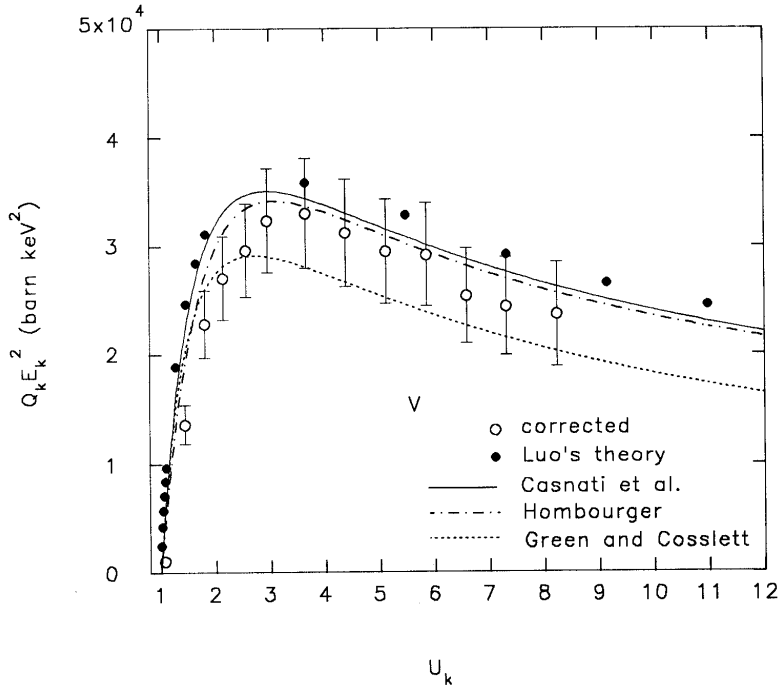

Figure 2. Plots of $Q_k E_k^2$ versus U_k for V; see also the caption to figure 1.

the experimental data of scandium and vanadium and of other elements measured before with the same method (i.e. Ti [9], Cr [6], Mn [7], Fe [7], Co [5], Ni [6], Cu [5], Zn [11], Nb [10] and Mo [8]).

In figures 1 and 2, the corrected cross sections of Sc and V are drawn and compared with the results given by the empirical formula of Casnati *et al* [25] and the calculated cross sections of Luo [13]. The measured data for these two elements are also compared with the results of the empirical formulae of Hombourger [16] and Green and Cosslet [28]. It can be seen that the corrected cross sections for Sc are in good agreement with the results of the semi-empirical formula of Green and Cosslet and are smaller than the predictions of the empirical formulae of Casnati *et al* [25] and Hombourger [16] and of Luo's theory [13], but for V the measured data are reasonably reproduced by the empirical formulae of Casnati *et al* [25] and Hombourger [16] and by the calculated cross sections of Luo [13].

In figure 3, the experimental data measured before with the same method for Ti, Cr, Mn, Fe, Co, Ni, Cu, Zn, Nb and Mo have been compared with the cross sections obtained from the empirical formula of Casnati *et al* [25] and the calculated cross sections of Luo [13]. For Cr, Fe, Co and Ni, the Casnati *et al* empirical formula and Luo's theory provide excellent agreement with the experimental data. Although the predictions of the Casnati *et al* empirical formula and Luo's theory are slightly higher than the experimental data for Mn and Cu, there is still acceptable agreement. For Ti and Zn, the Casnati *et al* empirical formula and Luo's theory do not agree well with the measured cross sections, especially for $U_k < 4$ for Ti. For Nb, the Casnati *et al* empirical formula overestimates the experimental data, but Luo's theory provides reasonable agreement. The Casnati *et al* empirical formula fits the experimental data very well for Mo for $U_k < 2$, while Luo's theory underestimates the experimental data. Moreover, the

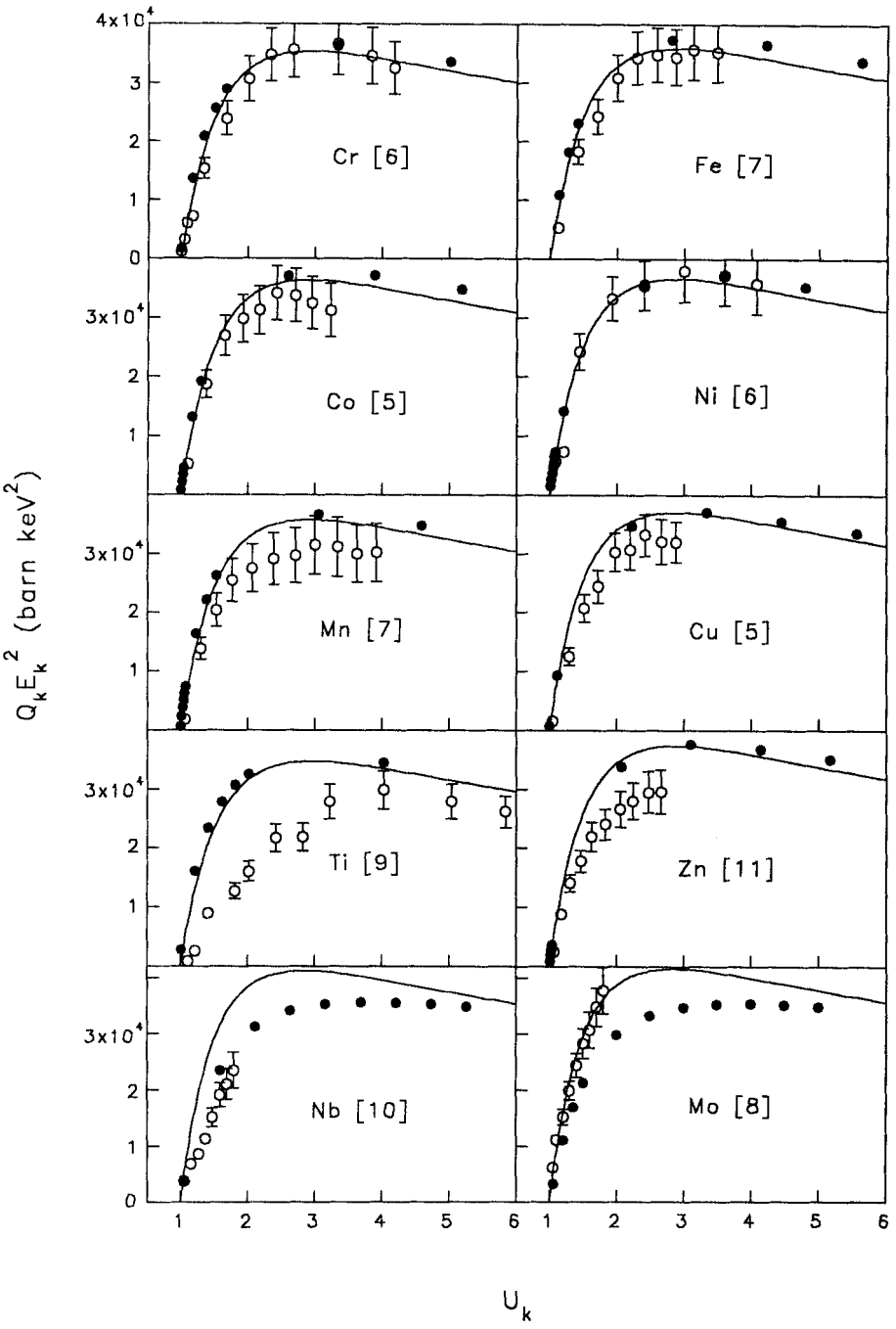

Figure 3. Plots of $Q_k E_k^2$ versus U_k for the elements. Hollow and solid circles represent the experimental data and Luo's theoretical results, respectively. The solid curves denote the results of the empirical formula of Casnati *et al*. An element symbol plus reference (for example, Cr [6]) indicates that the experimental data of this element (i.e. Cr) are taken from the corresponding reference (i.e. [6]).

experimental data for most elements analysed here always show a maximum for U_k near 2.5: this is consistent with the prediction of Bethe's theory, e.g. $Q_k E_k^2 \sim \ln U_k / U_k$, the maximum of the function $\ln U_k / U_k$ is reached at $U_k = e$. Overall, the Casnati *et al* empirical formula and Luo's theory can provide good or better agreement with the experimental data for the elements analysed here except for Sc, Ti and Zn. To some extent, this also implies that the experimental data measured with our method are reliable. Recently, Hombourger [16] has proposed an empirical formula based upon part of experimental data measured by Luo *et al* and some experimental data obtained by other groups.

In summary, in this paper, we have reported the experimental K-shell ionization cross sections of Sc and V at energies from near threshold to 45 keV. Comparison of the experimental data of scandium and vanadium and of other elements measured before with the same method (i.e. Ti, Cr, Mn, Fe, Co, Ni, Cu, Zn, Nb and Mo) with some empirical formulae and Luo's theoretical results has been made. It is shown that in general the empirical formula of Casnati *et al* and Luo's theory can provide good or better agreement with the experimental data for most of the elements analysed in the present paper.

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