PHOTOELECTRIC CROSS SECTION AND MASS ATTENUATION COEFFICIENT FOR Cu, Co, Ni AND CoCu, CoCuNi ALLOYS USING FERMI-THOMAS MODEL

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ABSTRACT

K-shell photoelectric effect cross sections were calculated for the elements Co, Cu and Ni, in the energy range from 10 keV to 30 keV. The method used was based on the use of nonrelativistic treatment for the electron in screening Coulomb potential. Fermi-Thomas model was used to represent the screening potential. Schrödinger equation could be solved accurately in spherical coordinates. The normalization of the continuum state wavefunction was obtained using Wentzel, Kramers and Brillowin (WKB) approximation. The results were given analytically and compared with the full relativistic screened calculations of Scofield. The mass attenuation coefficient was calculated for the CoCu, CoCuNi alloys and the results were compared with the experimental values reported by Seven. The results of this method were less accurate than those based on other methods like the self consistent field model for the atom. The value of this method lies in its simplicity and it can be presented analytically. The large difference between Seven and the theoretical ones was also investigated.

ABSTRAK

Keratan rentas bagi kesan fotoelektrik petala-K telah dihitung untuk unsur Co, Cu dan Ni, dalam julat tenaga 10 keV hingga 30 keV. Kaedah yang digunakan berdasarkan kepada penggunaan pendekatan ketidakrelatifan untuk elektron dalam keupayaan Coulomb tabir. Model Fermi-Thomas digunakan untuk mewakili keupayaan tabir. Persamaan Schrödinger telah diselesaikan dengan tepat dalam sistem koordinat sfera. Penormalan fungsi gelombang keadaan kontinum telah diperoleh dengan menggunakan penghampiran Wentzel, Kramers and Brillowin (WKB). Keputusan telah diberikan secara analisis dan telah dibandingkan dengan pengiraan kerelatifan ditabir daripada Scofield. Pekali pengecilan jisim telah dihitung untuk aloi CoCu, CoCuNi dan keputusan telah dibandingkan dengan nilai dapatan eksperimen seperti dilaporkan oleh Seven. Keputusan mengikut kaedah ini kurang tepat daripada kaedah lain seperti model medan konsisten diri untuk atom. Kelebihan kaedah ini adalah ia mudah dan boleh dinyatakan secara analisis. Perbezaan besar nilai yang dikira oleh Seven dengan nilai teori ini juga telah dikaji.

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LIST OF SYMBOLS

m	-	The mass of the electron
e	-	The charge of the electron
a_0	-	The radius of the hydrogen atom
$V(\rho)$	-	The potential energy of the electron at the distance ρ (in Rydberg units) from the nucleus
$U(\rho)$	-	The screening potential
Z	-	Atomic number
l	-	The azimuthal quantum number
m	-	Magnetic quantum number
$F(\beta, \gamma, x)$	-	Confluent hypergeometric function
R	-	Radial part of Schrödinger equation
N	-	Normalization factor
δ	-	Dirac delta function
M_{fi}	-	Matrix element
ω	-	The energy of the electron in Rydberg units
p	-	The momentum of the electron
α	-	Fine structure
N_A	-	Avogadro's number

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CHAPTER 1

INTRODUCTION

1.1 Main concepts

When a beam of photons (X- or gamma-rays) is allowed to pass through a material, it is subjected to an exponential reduction in its intensity. If I is the intensity of the beam at depth x and as it passes a distance dx in the material its intensity is reduced by an amount $-dI$, then the linear attenuation coefficient can be defined as

$$\mu = \frac{-dI / I}{dx}$$

Since the absorption depends on the quantity of material rather than the distance it travelled in the medium, it is important to divide this quantity (the linear attenuation coefficient μ) by the density ρ of the material. The result μ/ρ is called mass attenuation coefficient, here μ/ρ is measured by cm^2/g (Grodstein, 1957; Hubbell, 1969).

The mass attenuation coefficient μ/ρ is connected to the total cross section by the relation $\mu/\rho = (N_A/A)\sigma_t$, where N_A is the Avogadro's number and A is the atomic weight (Storm et al., 1970). The total cross section σ_t is the probability that a photon will be removed by all mechanisms of photon interaction with matter (Grodstein, 1957). In the energy range between 10 keV to 30 keV, photon can be removed by absorption (via photoelectric effect) or by scattering (via coherent or incoherent scattering), the contribution of scattering process to the total cross section is very small (not more than 2% of the total cross section) (Hubbell, 1969). For this reason

we neglect both coherent and incoherent scattering from our calculation and the concentration will be only on photoelectric effect.

1.2 Background information

The work in photoelectric effect started nonrelativistically in point Coulomb potential. This approach was worked by Stobbe (Hall, 1936; Pratt et al., 1964). The results are in agreement with the experiments in the energy range where $\hbar\omega << mc^2$ (i.e. in non-relativistic region). In the energy range for which $\hbar\omega >> I$, where I is the ionization energy of the electron, the problem is solved relativistically in point (unscreened) Coulomb potential by many authors like Hulme et al. (1935), Pratt (1960a). In the energy range that is in the neighborhood to the ionization energy, neither relativistic nor nonrelativistic results should be expected to be hold since the assumption that the screening effect are neglected is not valid. Scofield (1973) solved this problem relativistically where the electrons are assumed to be moving in the same Hartree-Slater central potential in both bound and continuum states. Manson and Cooper (1968) proposed a different solution for this problem, they solved it nonrelativistically using Hermann-Skillman central potential to represent screening, and the results were presented numerically for aluminum Z = 13.

In the present work the problem of photoelectric effect near the edge is also solved nonrelativistically, but the electron is supposed to be moving in Fermi-Thomas potential to represent screening.

1.3 Problem statement

In the hydrogen like atom, which was used widely in the early theoretical studies, the atom is supposed to be composed of a single electron in K-shell and a nucleus having a charge *Ze* (Hall, 1936; Pratt et al, 1973). According to this assumption, the theoretical value of the ionization energy is equal to Z^2R_y where R_y is the Rydberg energy (R_y =13.6 eV). But in reality, electrons in the outer shells screens (repel) the electrons in K-shell and thereby diminish the ionization energy. This means that, the observed ionization energy *I*(obs.) is less than the quantity Z^2R_y which is derived theoretically considering the atom is stripped from all other electrons (Hall, 1936). The difference ΔI between *I*(obs.) and the theoretical one effects on the calculations of photoelectric effect as follows; When the energy of photon is large enough to neglect ΔI the hydrogen like atom model is adequate and the results according of this model are in good agreement with the experimental ones (Jackson and Hawkes, 1981). When the energy of the incident photon is very close to the K-edge, ΔI cannot be neglected and the theoretical results which are based on the hydrogen-like atom model deviate from the experimental ones (Hall and Oppenheimer, 1931). There is also another problem arises when we apply this model on the photons whose energies lie between *I*(obs.) and Z^2R_y, because these photons, theoretically, unable to extract electrons from the K-shell while practically it is able to do so (Hall, 1936).

The effect of the molecular, chemical and crystalline environments on the absorption coefficients in the range and the alloys of interest are also investigated. Theoretically, these effects are very small (Grodstein, 1957) and accordingly the mixture rule can be adequate. Seven et al (2004) presented data showing a significant difference between experimental measurements of the mass coefficient and theoretical ones and according to the authors the reason of this difference is the factors mentioned above. This problem is discussed in this work.

Only for the comparison purposes, the elements and alloys and also the energy range used in this work were chosen to be similar to that presented

experimentally by Seven (2004). In Chapter 4, the values of energies used in this study were similar to those earlier used and presented in Seven (2004) for experimental considerations, while Scofield (1976) provided energies values for numerical work (Jackson and Hawkes, 1981).

1.4 Research objective

- To calculate the photoelectric effect cross section for three pure elements Co, Cu, Ni using nonrelativistic model in Fermi-Thomas screened Coulomb potential in the energy range from 10 keV to 30 keV.
- To calculate the mass attenuation coefficients for Co, Cu and Ni and alloys CoCu and CoCuNi using mixture rule.

1.5 Scope

In the present work, the photoelectric cross section is computed for the K-shell only for the pure elements Co, Cu and Ni at four values of energies in the energy range from 10 keV to 30 keV. The total atomic photoelectric effect is calculated using 5/4 rule which states that the total photoelectric effect cross section equals 5/4 times of the K-shell cross section. The results will be compared with the numerical ones in Scofield (1973). (Because of uncertainties in some experimental data we use the data of Scofield (1973) tabulation to provide data against which to test the validity of the various approximation.)

Although the data presented and discussed in this work concern the K-shell photoelectric effect cross sections, we also, for the completeness, calculate the total atomic cross section and the mass attenuation coefficients for the elements mentioned above. The mixture rule is also used to calculate the mass attenuation coefficients for the alloys CoCu and CoCuNi to estimate the effect of chemical bonds

and crystalline environments on the absorption of radiation. The results will be compared to the experimental ones of Seven (2004), and with the theoretical ones of Hubbell (1995).

In the energy range of interest, both coherent and incoherent scattering cross sections are very small. We will ignore them and we will consider the total atomic cross section equal to the photoelectric effect cross section only.

1.6 Software Used

Software that has been used in carrying out the calculations in this work is called MAPLE version 7, the software was developed in 1980 by the Symbolic Computer Group in the University of Waterloo.

Maple is a computer algebra system. There are many versions that have been released; the current major one is version 18 which was released in March 2014.

1.7 The organization of this work

The present work then is organized as follows; in chapter 2 the non-relativistic treatment of the electron using unscreened Coulomb potential is discussed, the work of the screened Coulomb potentials using different atomic model also are discussed. In chapter 3, the method used in this for treating photoelectric effect is discussed. Calculations and discussions have been presented in chapter 4. Finally, conclusions are presented in chapter 5.

REFERENCE

Alling, W. R., and Johnson, W. R. (1965). Exact Calculation of K-Shell and L-Shell Photoeffect. *Physical Review,* 139(4A), A1050-A1062.

Asher, J., Jones, O., Noyes, J., and Phillips, G. (1995). Kaye & Laby's Tables of Physical and Chemical Constants. Harlow: Longman.

Berestetskii, V. B., Lifshitz, E. M., and Pitaevski, L. P. (1971). Relativistic quantum theory (First edition ed.). Oxford: Pergamon Press.

Clark, H. (1982). *A first course in quantum mechanics* (2nd ed.). New York: Van Nostrand Reinhold.

Gavrila, M. (1959). Relativistic K-Shell Photoeffect. *Physical Review,* 113(2), 514-526.

Grodstein, G. R. (1957). X-ray Attenuation Coefficients From 10 keV to 100 MeV. *NBS* (583).

Hall, H. (1936). The Theory of Photoelectric Absorption for X-Rays and γ-Rays. *Reviews of Modern Physics,* 8(4), 358-397.

Hall, H., and Sullivan, E. C. (1966). K-Shell Photoelectric Cross Sections for the Fermi-Thomas Potential from 300 keV to 1.3 MeV. *Physical Review,* 152(1), 4-9.

Heitler, W. (1960). *The Quantum Theory Of Radiation* (3d edition ed.). London: Oxford Clarendon Press.

Hubbell, J., and Seltzer, S. (1995). Tables of X-ray mass attenuation coeffcients and mass energy-absorption coeffcients 1 keV to 20 MeV for elements Z = 1 to Z = 92 and 48 additional substances of dosimetric interest. *National Institute of Standarts and Physics Laboratory*, *NISTIR* (5632).

Hubbell, J. H. (1969). Photon cross section, attenuation coefficients, and energy absorption coefficients from 10 keV to 100 GeV. *NSRDS-NBS* 29.

Hubbell, J. H. (1982). Photon mass attenuation and energy-absorption coefficients from 1 KeV to 20 MeV. *International Journal of Applied Radiation.* 33 , 1269-1290.

Hubbell, J. H. (1999). Review of photon interaction cross section data in the medical and biological context. *Physics in Medicine and Biology*, 44, R1-R22.

Hubbell, J. H. (2006). Review and history of photon of cross section calculations. *Physics in Medicine and Biology,* 51, R245-R262.

Hulme, H. R., McDougall, J., Bukkinggham, A., Fowler, R. H. (1935). the photoelectric absorption of gamma rays in heavy elements. *Proceedings of Royal Society of London* A (149), 131.

Ibrahim, H., Hasan, K., and Mehmet, S. (2011). Determination of mass attenuation coefficients for natural minerals from different places of Turkey. *International Journal of the Physical Sciences,* 6(20), 4798-4801.

Jackson, D. F., and Hawkes, D. (1981). X-ray attenuation coefficients of elements and mixtures. *Physics Reports,* 70(3), 169-233.

Johnson, A. (1965). *Quantum Mechanics Non-relativstic Theory* (2nd ed.). London: Pergamon Press Ltd.

Manson, S. T., and Cooper, J. W. (1968). Photo-Ionization in the Soft x-Ray Range: 1Z Dependence in a Central-Potential Model. *Physical Review,* 165(1), 126-138.

Matese, J. J., and Johnson, W. R. (1965). Influence of Screening on the Atomic Photoeffect. *Physical Review,* 140(1A), A1-A7.

McEnnan, J., Kissel, L., and Pratt, R. H. (1976). Analytic perturbation theory for screened Coulomb potentials: Nonrelativistic case. *Physical Review A,* 13(2), 532-559.

McGuire, E. J. (1968). Photo-Ionization Cross Sections of the Elements Helium to Xenon. *Physical Review,* 175(1), 20-30.

Murty, V. R. K., and Devan, K. R. S. (1997). Atomic Photoeffect Below 100 keV. *Applied Radiation and lsotopes,* 48, 1501-1506.

Oh, S. D., McEnnan, J., and Pratt, R. H. (1976). Analytic calculation of screened photoeffect cross sections. *Physical Review A,* 14(4), 1428-1436.

Pratt, R. H. (1960a). Atomic Photoelectric Effect at High Energies. *Physical Review,* 117(4), 1017-1028.

Pratt, R. H. (1960b). Photoeffect from the L Shell. *Physical Review,* 119(5), 1619-1626.

Pratt, R. H., Levee, R. D., Pexton, R. L., and Aron, W. (1964). K-Shell Photoelectric Cross Sections from 200 keV to 2 MeV. *Physical Review,* 134(4A), A898-A915.

Pratt, R. H., Ron, A., and Tseng, H. K. (1973). Atomic Photoelectric Effect Above 10 keV. *Reviews of Modern Physics,* 45(2), 273-325.

Rakavy, G., and Ron, A. (1967). Atomic Photoeffect in the Range E{γ}=1-2000 keV. *Physical Review,* 159(1), 50-56.

Scofield, J. H. *L. L. L.* (1973). Theoretical photoionization cross sections from 1 to 1500 keV. *Report UCRL* (51326).

Seven, S., H., I., Omer, K., and Bakkaloglu, F. (2004). The Measurement of Mass Attenuation Coefficients of CoCu, CoCu Ni alloys. *Journal of Quantitative Spectroscopy and Radiative Transfer,* 83, 237-242.

Sneddon, I. N. (1956). Special functions of mathematical physics and chemicals. Edinburgh: Oliver & Boyd.

Storm, E., Harvey, and Israel, I. (1970). Photon cross sections from 1 keV to 100 MeV for elements Z=1 to Z=100. *Atomic Data and Nuclear Data Tables, 7*(6), 565-681.

Thomas, L.H. (1927). *the calculation of atomic fields.* paper presented at the mathematical proceedings of the cambribge philospphical society.