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On the effective atomic number and electron density: A comprehensive set of formulas for all types of materials and energies above 1 keV

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Dedicated to the memory of John H. Hubbell (1925–2007).

Abstract

A comprehensive and consistent set of formulas is given for calculating the effective atomic number and electron density for all types of materials and for all photon energies greater than 1 keV. The formulas are derived from first principles using photon interaction cross sections of the constituent atoms. The theory is illustrated by calculations and experiments for molecules of medical and biological interest, glasses for radiation shielding, alloys, minerals and liquids.

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1. Introduction

The atomic number, Z, is a ubiquitous parameter in atomic and nuclear physics where it occurs in almost any formula. For a complex medium, the effective atomic number, Z_{eff}, is in some cases a convenient parameter for representing X-ray and gamma ray interactions, e.g. in designs of radiation shielding or in calculations of absorbed dose in radiotherapy. However, as stated by Hine [1], a single number cannot represent the effective atomic number of a material, which is composed of several elements. For each of the different processes, by which X-rays and gamma rays can interact with matter, the various atomic numbers in the material have to be weighted differently. Accordingly, Z_{eff}, is no true constant for a given material, but a parameter varying with photon energy depending on the interaction processes involved. The effective atomic number is closely related to the electron density, expressed in number of electrons per unit mass.

Early calculations of the effective atomic number were based on parameterization of the photon interaction cross section by fitting data over limited ranges of energy and atomic number [2]. As the present results will show, accurate databases of photon interaction cross sections and interpolation programs, e.g. [3–5], have made it possible to calculate Z_{eff} with much improved accuracy and information content over a wide range of photon energy. This will be illustrated by calculations for bio-molecules, glasses, alloys, minerals and liquids. Wherever possible, the results are compared with experimental data.

Among early applications one may mention bone densitometry and measurements of fat content in liver [6]. Yang

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et al. [7] measured Z_{eff} of soft human tissues, such as blood, brain, heart, and liver. Kumar and Reddy [8] determined the effective atomic number for some materials of dosimetric interest. Singh et al. [9–12] determined the effective atomic numbers for several glasses with potential use in radiation shielding.

Recently, Manjunathaguru and Umesh [13,14], Manohara and Hanagodimath [15,16], Manohara et al. [17], and Kumar et al. [18] have determined the effective atomic number of several molecules with a variety of roles in biochemistry. Grinyov et al. [19] have developed dual-energy radiography for separate detection of materials differing in their effective atomic number and local density. Similarly, Torikoshi et al. [20] have developed a dual-energy X-ray CT method using synchrotron radiation to obtain high-resolution Z_{eff} images that can be used for medical diagnosis.

It follows from above that there is a renewed interest in the effective atomic number as a parameter for characterizing the X-ray and gamma ray response of materials, particularly for applications in radiation shielding, dosimetry, biology and medicine. Various formulas and approaches have been used in the past for calculating Z_{eff}, but there seems to be a need for a comprehensive and consistent set of formulas, derived from first principles and valid for all types of materials and for all photon energies greater than 1 keV. The aim of the present paper is to fill this gap in the literature.

2. Basic formulas

Consider first a chemical compound. The formulas will later be generalized to mixtures as well. The total photon interaction cross section, σ_{m}, per molecule can be written

$$\sigma_{\text{m}} = \sum_i n_i \sigma_i, \tag{1}$$

where n_i is the number of atoms of the ith constituent element, and σ_i is total photon interaction cross section per atom of element i. The total number, n, of atoms in the molecule is

$$n = \sum_i n_i. \tag{2}$$

Suppose that the cross section per molecule can be written in terms of an effective (average) cross section, σ_{a}, per atom and an effective (average) cross section, σ_{e}, per electron as follows:

$$\sigma_{\text{m}} = n\sigma_{\text{a}} = nZ_{\text{eff}}\sigma_{\text{e}}. \tag{3}$$

Eq. (3) can be regarded as the definition of the effective atomic number. Essentially, it assumes that the actual atoms of a given molecule can be replaced by an equal number of identical (average) atoms, each of which having Z_{eff} electrons.

It follows from the first equality of Eq. (3) that the effective (average) cross section per atom is given by

$$\sigma_{\text{a}} = \frac{1}{n}\sum_i n_i \sigma_i. \tag{4}$$

Similarly, the effective (average) cross section per electron is given by

$$\sigma_{\text{e}} = \frac{1}{n}\sum_i n_i \frac{\sigma_i}{Z_i}. \tag{5}$$

It follows from the last equality of Eq. (3) that the effective atomic number can be written as the ratio between the atomic and electronic cross sections:

$$Z_{\text{eff}} = \frac{\sigma_{\text{a}}}{\sigma_{\text{e}}}. \tag{6}$$

Many authors have used Eq. (6) for calculating Z_{eff}. However, it is instructive to go one step further and insert the expressions (4) and (5) for σ_{a} and σ_{e}:

$$Z_{\text{eff}} = \frac{\sum_i n_i \sigma_i}{\sum_j n_j \frac{\sigma_j}{Z_j}}. \tag{7}$$

Eq. (7) is then the basic relation for calculating the effective atomic number of a chemical compound, and it will be further elaborated in the following. It may be noted in passing that Eq. (7) can be rewritten as

$$\frac{1}{Z_{\text{eff}}} = \frac{\sum_i n_i \sigma_i \frac{1}{Z_i}}{\sum_j n_j \sigma_j}. \tag{8}$$

Eq. (8) shows that $(1/Z_{\text{eff}})$ is the weighted arithmetic mean of $(1/Z_i)$, where the weighting factor associated with each element is $n_i\sigma_i$. For each of the different processes, by which photons can interact with matter, the weighting factor is different, because of the different Z dependence of the atomic cross section.

Eq. (7) has been derived for a chemical compound, assuming that each n_i is an integer. A more general expression for Z_{eff} can be obtained by introducing the molar fraction, f_i (sometimes expressed in units of atomic percent, at.%). For a chemical compound one has

$$f_i = \frac{n_i}{\sum_j n_j} = \frac{n_i}{n}, \tag{9}$$

where $\sum_i f_i = 1$. Rewriting Eq. (7) in terms of molar fractions gives the more general expression

$$Z_{\text{eff}} = \frac{\sum_i f_i \sigma_i}{\sum_j f_j \frac{\sigma_j}{Z_j}}. \tag{10}$$

Eq. (10) is then the basic relation for calculating the effective atomic number for all types of materials, compounds as well as mixtures.

2.1. Compton scattering

Compton scattering is the main interaction process for low- and medium-Z elements in a certain energy range, typically between 0.05 and 5 MeV. In passing, it should be remarked that for high-Z elements there is no energy region where Compton scattering is totally dominating.