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Concept of effective atomic number and effective mass density in dual-energy X-ray computed tomography

Anne Bonnin [a,b], Philippe Duvauchelle [b,*], Valérie Kaftandjian [b], Pascal Ponard [c]

[a] ESRF, 6 Jules Horowitz, F-38073 Grenoble Cedex, France
[b] LVA, Vibrations and Acoustic Laboratory, INSA-Lyon, Université de Lyon, F-69621 Villeurbanne Cedex, France
[c] Thales Electron Devices SAS, 2 Rue Marcel Dassault, BP23 78141 Vélizy, Villacoublay Cedex, France

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ABSTRACT

This paper focuses on dual-energy X-ray computed tomography and especially the decomposition of the measured attenuation coefficient in a mass density and atomic number basis.

In particular, the concept of effective atomic number is discussed. Although the atomic number is well defined for chemical elements, the definition of an effective atomic number for any compound is not an easy task. After reviewing different definitions available in literature, a definition related to the method of measurement and X-ray energy, is suggested. A new concept of effective mass density is then introduced in order to characterize material from dual-energy computed tomography.

Finally, this new concept and definition are applied on a simulated case, focusing on explosives identification in luggage.

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1. Introduction

X-ray computed tomography (CT) is a well known 3D technique which enables one to determine a local value of the linear attenuation coefficient μ of a material. This coefficient depends on the X-ray energy and the characteristics of the material (its mass density ρ and its atomic number Z). Nevertheless, different materials can have the same attenuation coefficient at a given energy. For this reason, dual-energy techniques have been introduced. First applied in the medical field, they have also been used in radioscopy mode for industrial applications, amongst others in luggage inspection.

From the measurements acquired at two different energies, different choices have been proposed in the literature to differentiate two or more materials. The first approach, described by Alvarez et al. [1] and Macowski et al. [17], was to express μ as a function of mass density and atomic number. Thus using two energies, it is possible to derive a (ρ,Z) couple from the two measured attenuation coefficients. Other approaches showed that an unknown material can be expressed as a linear combination of two components forming a reference basis. These components can be, for example, the two physical contributions resulting from photoelectric absorption and Compton scattering or two reference materials used during a calibration step (see [16]). For example, these two materials can be bone and soft tissue [15], while in the industrial field plexiglass and iron can be chosen for radioactive waste drums inspection [23,22].

The discrimination of materials based on atomic numbers and mass densities, as proposed originally by Alvarez, is mainly used in luggage inspection and enables one to differentiate organic from inorganic materials, or more precisely, light from heavy materials.[1] A calibration process is also needed, from two to a set of different materials [3]. In this case, materials are classified in categories (light vs. heavy) but not really identified.

Our article is based on the decomposition of μ in a (ρ,Z) basis, whose principle is described in Section 2. A question arises then: what is the meaning of the atomic number for a compound[2] of several chemical elements (which is the case of most common materials)?

After reviewing several Z_{eff} definitions in the third section, we propose our own definition in Section 4, in which Z_{eff} depends on the energy. Therefore, in the context of dual-energy measurement, we show in Section 5, that it is necessary to introduce also the concept of effective mass density ρ_{eff}. Hence any material is characterized by a unique (ρ,Z) couple for the given couple of energies. In Section 6, the influence of both energies is studied for water. In the last part of this article, our method has been used on a phantom in the context of explosives detection.

* Corresponding author. Tel.: +33 4 72 43 70 58.
E-mail addresses: annebonnin@free.fr (A. Bonnin), philippe.duvauchelle@insa-lyon.fr (P. Duvauchelle).

[1] The frontier between light and heavy materials is considered to be situated at $\rho \sim 2$ g cm^{-3} and $Z \sim 8$.

[2] In this publication, we will use the term "compound" to refer to any sample with more than one chemical element such as chemical compounds, mixtures, alloys, etc.…

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2. Theoretical background

In CT, materials are differentiated thanks to their linear X-ray attenuation coefficient μ. Following Alvarez et al. [1], for a given energy E, μ is a function of the mass density ρ and atomic number Z of the element as follows:

$$\mu_E(\rho,Z) = \alpha_E \rho Z^{m_E} + \beta_E \rho. \quad (1)$$

In order to determine ρ and Z at each point of the sample, the use of two energies (a low energy *LE* and a high energy *HE*) is needed to solve the equation system:

$$\begin{cases} \mu_{LE} = \alpha_{LE}\rho Z^{m_{LE}} + \beta_{LE}\rho \\ \mu_{HE} = \alpha_{HE}\rho Z^{m_{HE}} + \beta_{HE}\rho \end{cases} \quad (2)$$

The dual-energy CT method is realized in two steps.

The first step consists of a calibration with a sample of known materials (ρ,Z), in order to obtain the coefficients α_{LE}, m_{LE}, β_{LE} and α_{HE}, m_{HE}, β_{HE} (see Eq. (2)) and then the two calibration surfaces: $\mu_{LE} = f(\rho,Z)$ and $\mu_{HE} = g(\rho,Z)$.

The second step consists in a measurement of μ at two energies for an unknown material. The (ρ,Z) couple of this material can then be deduced by solving Eq. (2). For an element, there is no ambiguity on the determination of Z. But for a compound, the concept of effective atomic number is widely discussed in the literature and we cannot find a unique definition well accepted by the research community. In the following section, we review some existing definitions.

3. Review of existing methods to define Z_{eff}

Different calculation methods can be found in the literature to define the effective atomic number Z_{eff} for a compound. These expressions are presented below. Some of them have already been collected by [7].

They can be classified in two categories. The first one is based on calculations involving the atomic number Z_i of the ith atom constituting the compound and for some of them, their validity field depends on the X-ray energy. The second category gathers the methods based on mass attenuation coefficients.

3.1. Z_{eff} obtained from calculation methods

Z_{eff} can be considered in a general way as a function of atomic numbers Z_i weighted by the percentages of each element i in the compound. For an element i, the atomic number Z_i represents the number of protons or electrons contained in the corresponding atom.

Considering absorption in biological materials such as organs, Spiers in 1946 [26], established an expression of the effective atomic number according to the percentage of electrons α_i^e:

$$Z_{eff\,1} = \left[\sum_i \alpha_i^e Z_i^{2.94}\right]^{1/2.94} \quad \text{with} \quad \alpha_i^e = \frac{n_i Z_i}{\sum_i n_i Z_i} \quad (3)$$

where n_i is the number of atoms.

One year later, in the radiological field, Glasser [10] established the following expression directly based on the mass percentage ω_i:

$$Z_{eff\,2} = \left[\frac{\sum_i \omega_i Z_i^4}{\sum_i \omega_i Z_i}\right]^{1/3} \quad (4)$$

where A_i is the atomic mass, ω_i the mass percentage of each element i expressed as a function of n_i and A_t the total atomic mass of the compound:

$$\omega_i = \frac{n_i A_i}{A_t} \quad (5)$$

In 1952, Hine [13] introduced an expression of Z_{eff} as a function of each specific interaction process but only for the photoelectric effect, $Z_{eff\,3a}^{3.1} = \sum_i \omega_i Z_i^{3.1}$, and for the pair creation, $Z_{eff\,3b} = \sum_i \omega_i Z_i$. After comparison of this study, giving substantially the same results for different compounds for these two partial processes, Murty [19] assumed that the effective atomic number can be approximated by a unique relation, defined in Eq. (6), valid also for the Compton effect at intermediate energies:

$$Z_{eff\,4} = \frac{\sum_i \frac{\omega_i Z_i}{A_i}}{\sum_i \frac{\omega_i}{A_i}}. \quad (6)$$

Tsai and Cho [27] reviewed Spiers equation (Eq. (3)), by revaluing the power factor from 2.94 to 3.4 on the basis of attenuation measurements carried out on biological tissues. This time, the expression is valid only for energies lower than 150 keV:

$$Z_{eff\,5} = \left[\sum_i \alpha_i^e Z_i^{3.4}\right]^{1/3.4} \quad (7)$$

To characterize organic matter (i.e. light elements with $Z < 10$) at energies greater than 20 keV, Schätzler [24], applied the relation proposed by Hine for pair creation, where the atomic number Z_i of each element i, is weighted by the mass percentage ω_i of this element:

$$Z_{eff\,6} = \sum_i \omega_i Z_i \quad (8)$$

Later, on a limited range of Z, Manninen, and Koikkalainen [18] suggested a relation introducing the percentage of atoms α_i^{at}:

$$Z_{eff\,7} = \left[\frac{\sum_i \alpha_i^{at} Z_i^3}{\sum_i \alpha_i^{at} Z_i}\right]^{1/2} \quad \text{with} \quad \alpha_i^{at} = \frac{n_i}{\sum_i n_i}. \quad (9)$$

Puumalainen [21] then simplified the relation as:

$$Z_{eff\,8} = \sum_i \alpha_i^{at} Z_i. \quad (10)$$

This list of calculation methods is not thorough. This illustrates that for each specific need, a particular method is applied, according to the range of energy, the type of compounds, the field of application.

3.2. Z_{eff} obtained from mass attenuation coefficients database

Guru Prasad et al. [12] proposed a way to find the effective atomic number for a compound at a given energy: for a series of alloys, assuming that the photoelectric absorption is predominant between 10 and 150 keV, and knowing the tabulated mass attenuation coefficients of elements $\frac{\mu}{\rho}(Z,E)$ (see [14], [6] and the National Institute of Standards and Technology (NIST) reference data website, XCOM [2]), they calculate a so-called "cross-section per atom on average in the alloy" σ_a, first presented by Conner et al. [4] and defined for a compound by:

$$[\sigma_a]_{compound} = \frac{[(\mu/\rho)_{tabulated}]_{compound}}{N_A \sum_i \frac{\omega_i}{A_i}}. \quad (11)$$

From Eq. (11) and for the different elements, he obtains $\sigma_a = f(E)$ (as $\frac{\mu}{\rho}$ depends on E) and then for a given energy, $\sigma_a = f(Z)$. A linear interpolation of all these values provides a theoretical curve of σ_a depending on the atomic number Z for a given energy: $\sigma_a = f(Z_{eff})$. The effective atomic number of a compound, Z_{eff9}, is obtained graphically thanks to the intersection of this curve and the

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