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Element analysis and calculation of the attenuation coefficients for gold, bronze and water matrixes using MCNP, WinXCom and experimental data

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HIGHLIGHTS

- We used MCNP-4C code for simulation.
- We compared experimental and MCNP results for various matrixeses in different energies.
- We simulated mass attenuation coefficients and element analysis (EDXRF) for some matrixes.

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ABSTRACT

In this study, element analysis and the mass attenuation coefficient for matrixes of gold, bronze and water with various impurities and the concentrations of heavy metals (Cu, Mn, Pb and Zn) are evaluated and calculated by the MCNP simulation code for photons emitted from Barium-133, Americium-241 and sources with energies between 1 and 100 keV. The MCNP data are compared with the experimental data and WinXCom code simulated results by Medhat. The results showed that the obtained results of bronze and gold matrix are in good agreement with the other methods for energies above 40 and 60 keV, respectively. However for water matrixes with various impurities, there is a good agreement between the three methods MCNP, WinXCom and the experimental one in low and high energies.

1. Introduction

Impurities and trace elements affect on matrix mass attenuation coefficients. Different methods are used to analyze and determine the concentration of impurities such as destructive and non-destructive methods. Destructive method is the predominant method of determining the concentration of elements in solution. This method causes environmental pollution and may deteriorate the samples. But in non-destructive method, it is seen that the accuracy of detection is high and a much smaller number of samples are detected. Most nuclear techniques are non-destructive, highly sensitive rapid with minimum sample requirement.

Most of the nuclear methods used for elements analysis include: X-ray fluorescence (XRF) (Beckhoff et al., 2006; Jenkins and De Vries, 1973; Zoeger et al., 2006; Buhrke et al., 1998), proton induced X-ray emission (PIXE) (Manikandan, 2011; Ruvalcaba et al., 2001), electron spectroscopy for chemical analysis (ESCA) (Siegbahn et al., 1967; Feng et al., 1999) and instrumental neutron activation analysis (INAA) (Gordon et al., 1968; Lieser, 2001; Muecke, 1980) methods. Another of non-destructive method is the gamma-absorption one. This method is based on the attenuation of photons transmitted through the material. The advantage of the gamma absorption method over other methods is that this procedure is simple, rapid, inexpensive and practical. The radiation passes through a material to be attenuated exponentially, the attenuating of material is considered by the attenuation coefficient (μ and μ/ρ) in it. The expressions show the attenuation of beam intensity in different materials and the use of quantities shows that a decrease in beam intensity is the function of the environmentally effective Z number and photon energy (Midgley, 2005; Medhat, 2012a, 2012b; Jackson and Hawkes, 1981). Mass attenuation coefficient of the solid and liquid samples was calculated by software that designed first by Berger and Hubbell (1987)). The changes on the software were applied by Gerward et al. (2004)),

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and were updated in other software environment (Gerward et al., 2004).

One of the important non-destructive methods for finding the trace elements and impurities in a matrix is EDXRF (energy dispersive X-ray fluorescence). In EDXRF method, the sources that are used for determination of the impurities in a matrix include Americium-241 (Am-241) and Barium-133 (Ba-133). Americium-241 was discovered in 1945 in the United States. Isotope Am-241 was achieved in neutron reactions of the plutonium isotopes in a nuclear reactor in 1944. Alpha-ray activity of this element is three times greater than that of the radium element. Americium-241 is commonly used for low-energy gamma-ray sources. Barium metal is silver-white and naturally exists in the environment. Due to the extensive use of barium in the industry, many human activities have distributed barium in environment. One of the most widely used radioisotopes of this element is isotope 133, which has more than 9 energy levels of gamma rays and in EDXRF method is used to find the amount of impurities in the matrix.

MCNP-4C simulation code is a multi-purpose computational code with a continuous energy spectrum for reactor design and radiation shielding. This code is based on the Monte Carlo method to solve the transport equation; furthermore, it can work on different modes of delivery that are capable to consider neutrons, electrons and photons, alone, or in pairs all three together (Briesmeister, 2000).

Table 1
Composition of bronze and gold alloy sample (Medhat, 2012a, 2012b).

Bronze			Gold			
No.	Cu (%)	Sn (%)	Karat	Au (%)	Cu (%)	Ag (%)
BZ1	57	43	K14	58	28	**14**
BZ2	88	12	K18	75	3	**22**
BZ3	90	10	K21	91	2	**7**

Table 2
Comparison of MCNP, experimental and theoretical mass attenuation coefficients for gold and bronze alloys at 59.5 and 81 keV.

μ/ρ (cm^2 g^{-1})						
Energy	59.5 keV			81 keV		
	MCNP.	Exp.	Calc.	MCNP.	Exp.	Calc.
Bz_1	3.631	3.686	3.731	1.54	1.693	1.737
Bz_2	2.072	2.123	2.189	0.881	1.001	1.035
Bz_3	1.974	1.983	2.09	0.835	0.707	0.989
K_{14}	3.81	3.870	3.88	1.927	1.850	1.852
K_{18}	4.236	4.695	4.713	2.0	2.230	2.245
K_{21}	4.161	4.520	4.557	1.911	2.170	2.189

Table 3
Relative difference μ/ρ (cm^2 g^{-1}) of theoretical and experimental methods with MCNP method.

Relative difference (%)				
Energy	59.5 keV		81 keV	
	Exp.	Calcu.	Exp.	Calcu.
BZ1	1.52	2.75	9.94	12.79
BZ2	2.46	5.65	13.62	17.48
BZ3	0.46	5.88	15.33	18.44
K14	1.58	1.84	4.0	3.9
K18	10.84	11.26	11.5	12.25
K21	8.63	9.52	13.55	14.55

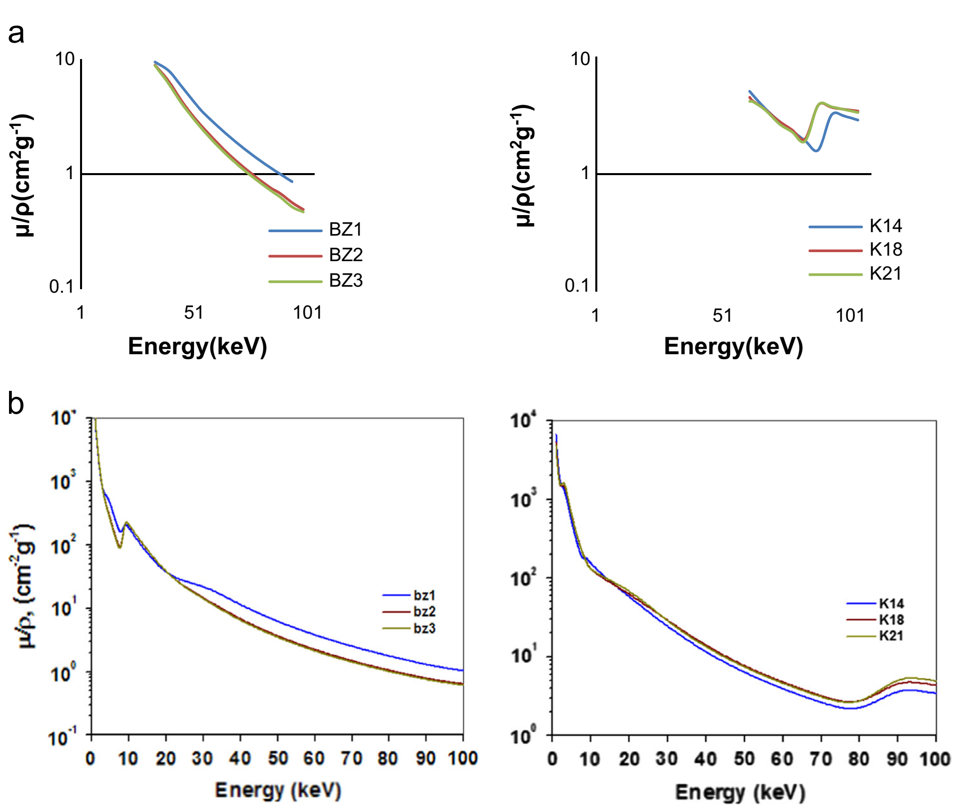

Fig. 1. The calculated mass attenuation coefficients for the investigated bronze and gold alloys in low energy range (1–100 keV). (a) Diaphragm calculated from MCNP simulation. (b) Diaphragm calculated from theoretical and experimental methods (Medhat, 2012a, 2012b).