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EFFECTIVE ATOMIC NUMBERS AND ELECTRON DENSITIES OF GEL DOSIMETERS FOR He, B, C, AND O HIGHLY CHARGED PARTICLES INTERACTION IN THE ENERGY RANGE 10 keV–100 MeV

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The radiological properties of different gel dosimeter formulations including six normoxic and four hypoxic polymeric gels, BRESAGE, PREAGE®, Fricke gel dosimeters, and water were investigated using SRIM code. The effective atomic number Z_{eff} and electron density (N_e) for heavily charged particle interaction were calculated and performed for Helium (He), Boron (B), Carbon (C), and Oxygen (O) ion interactions in the energy range from 10 keV to 100 MeV. Variations of effective atomic number (Z_{eff}) and electron density (N_e) with the kinetic energy of ions, (He, B, C, and O), were observed over the whole energy range for all studied materials. Variations of Z_{eff} for He ion are up to 21%, 25%, and 20% for hypoxic and normoxic gels, Fricke gel, and PRESAGE gels, respectively. For other ions, variation is up to 34% for hypoxic and normoxic gels as well as Fricke gel, and 32% for PRESAGE gels. It is found that the maximum values of Z_{eff} have been observed in intermediate energies between 1-10 MeV for all dosimeters, except for PRESAGE and PRESAGE®, where maximum values were observed in the relatively low energy range 10 – 100 keV. For effective atomic number relative to water, polymeric gels and Fricke gel showed better water equivalence with differences <7%, while PRESAGE and PRESAGE® showed high differences up to 17.5%, 22%, 21%, and 25% for He, B, C, and O ion, respectively. Gels found to be most relative to water are (Fricke, HEAG, and PAG), Fricke and HEAG), (Fricke and HEAG), and (Fricke, HEAG, and BANG-1) for He, B, C, and O ion interactions, respectively. Data reported here gives essential information about the interaction of different types of charged particles with different materials and could be useful in the energy range specified.

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Keywords: Effective atomic number, Electron density, Highly charged ions, Gel dosimeters, SRIM code

1. Introduction

Effective atomic number Z_{eff} and electron density N_e of materials are of the most convenient parameters that represent characteristics of multi-element materials for radiation interaction depending mainly on the atomic number of its constituent elements [1], which result in different radiation interaction probabilities in different energy ranges and the energy of incident radiation; hence, it could not be expressed with one single number. Since it is energy dependant parameter, it could be used to evaluate the radiological properties of compounds, mixtures, and composites. Atomic numbers Z_{eff} and N_e are widely used in radiation dosimetry, radiation therapy, medical diagnosis, and in many technical and medical fields.

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Polymeric gel dosimeters are fabricated from radiation-sensitive chemicals [2] which are polymerized as a function of radiation absorbed dose. It gains its importance from its ability to record radiation dose distribution in three dimensions compared to other types of dosimeters.

In the application of gel dosimetry, consideration of the radiological properties of these materials for different types of radiation in different energy regions is a very important issue. This importance increases with the increasing use of highly charged particles in medical applications, including both therapeutic and diagnostic. In literature, several studies of Z_{eff} in gel dosimeters are being carried out for photon [3] and electron interactions [4], but studies regarding highly charged particles are very few. Recently, a method adopted by Kurudirek [5–8] for calculation of effective atomic number for highly charged particle interaction has been used to investigate Z_{eff} for different materials, such as human tissues, dosimetric materials [9,10], vitamins, and biomolecules [5–6], [11,12].

No study is carried out regarding Z_{eff} and N_e of gel dosimeters for charged particle interaction except work done by Kurudirek [9] for a limited number of gels within limited energy range, thus this is the promotion behind this work.

The present study deals with calculations of the effective atomic number Z_{eff} and electron density N_e of gel dosimeters developed for 3D optical dosimetry, which includes Fricke gel, four hypoxic and six normoxic polymeric gel dosimeter formulations, PRESAGE gel, and PRESAGE®. The calculation is performed in the energy range 10 keV – 100 MeV for He, B, C, and O ion total interactions.

2. Materials and methods

The elemental composition of gel dosimeters studied is available for polymeric gels and Fricke gel in [3], PRESAGE gel [13], and PRESAGE® [14]. Their effective atomic number and electron density have been calculated for energy range 10 keV – 100 MeV, using the method adopted by Kurudirek [5–8] for highly charged particle interaction.

2.1. Stopping powers calculation

Mass stopping powers of constituent elements of the gel molecule were obtained using the Stopping and Range of Ions in Matter (SRIM) code [15-17], spanning the range from 10 keV to 100 MeV. The mass stopping power values for the selected gels were estimated using the mixture rule (Bragg's additive law) [18] and the elemental stopping of the constituent elements obtained above are as follows:

$$(S/\rho)_{gel} = \sum_{i=1}^{n} w_i (S/\rho)_i \quad (1)$$

where $(S/\rho)_i$ is the mass stopping of i^{th} element in the molecule of gel, n is the number of constituent elements and w_i is the weight fraction of the i^{th} element in a molecule of gel so that

$$\sum_{i=1}^{n} w_i = 1 \quad (2)$$

2.2. Stopping cross-sections (σ_{gel})

Stopping cross-sections were obtained by dividing the mass stopping power of the gel by the total number of atoms present in one gram of the gel:

$$\sigma_{gel} = \frac{(S/\rho)_{gel}}{N_A \sum_i (w_i/A_i)} (barn/atom) \quad (3)$$

where N_A (= 6.022 x 10^{23}) is Avogadro's number in atom g^{-1}, w_i is the weight fraction of the i^{th} element in a molecule of gel, and A_i is the atomic weight of i^{th} element in the molecule.

2.3. Z_{eff} calculation

The Z_{eff} values were calculated by the logarithmic interpolation of Z values between the adjacent stopping cross-section data as follows:

$$Z_{eff} = \frac{Z_1(\log\sigma_2 - \log\sigma \quad) + Z_2(\log\sigma - \log\sigma_1)}{\log\sigma_2 - \log\sigma_1} \tag{4}$$

where (σ) is the cross-section of the material, σ_1 and σ_2 are the elemental cross-sections between which the stopping cross-section of the material lies, and Z_1 and Z_2 are the atomic numbers of the elements corresponding to σ_1 and σ_2, respectively.

2.4. Electron density N_e

The electron density of the gels has been calculated using the following formula:

$$N_e = Z_{eff}\, N_A/\langle A\rangle\, (electrons/g) \tag{5}$$

where N_A is the Avogadro's number and $\langle A\rangle$ is the relative atomic mass of the gel.

3. Results and discussion

Since Z_{eff} and N_e values were derived from mass stopping power data, accuracy in Z_{eff} values are due to the accuracy in stopping powers calculation using SRIM code, which is stated to be 3.9%, 3.5%, 4.6%, and 5.6% for H ion, He ion, Li ions, and (Be-U), respectively, with an overall accuracy of 4.3% [15]. The obtained values of Z_{eff} and N_e for selected energy values for the different ions are presented in Fig.1 to Fig.8. Table1 shows basic statistical information of the effective atomic numbers for all ions studied. Figure 1 below shows that variation in Z_{eff} and N_e values have been observed through the entire energy range (10 keV–100 MeV) for all types of charged particles studied.

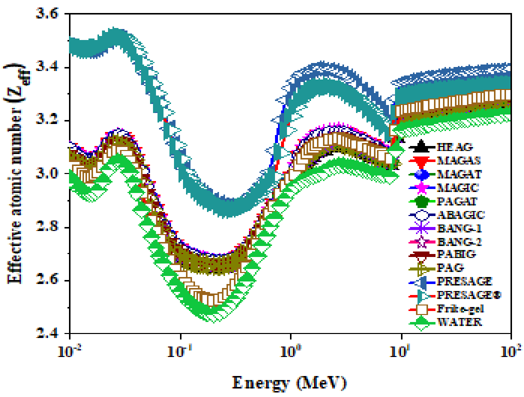

Fig. 1. Variation of effective atomic number Z_{eff} of dosimetric gels with the kinetic energy of He ion.

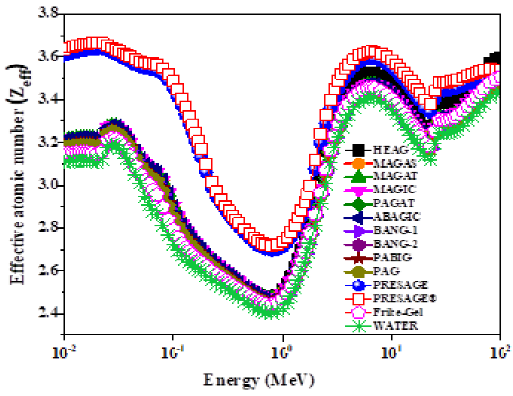

Fig. 2. Variation of effective atomic number Zeff of dosimetric gels with the kinetic energy of B ion.

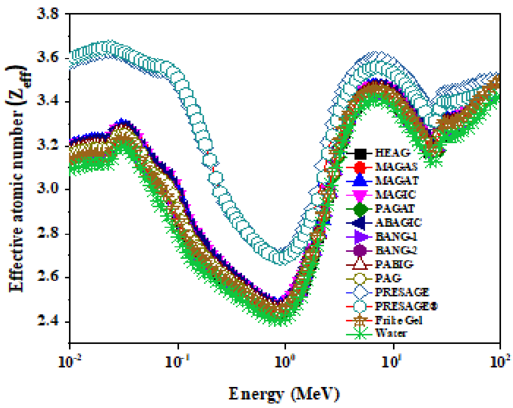

Fig. 3. Variation of effective atomic number Zeff of dosimetric gels with the kinetic energy of C ion.

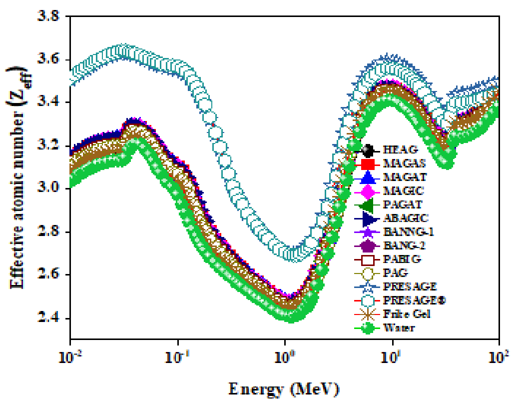

Fig. 4. Variation of effective atomic number Zeff of dosimetric gels with the kinetic energy of O ion.

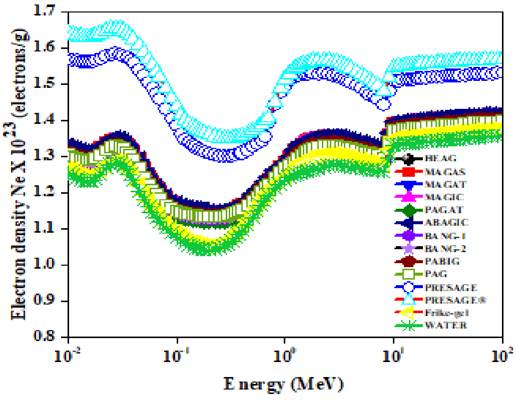

Fig. 5. Variation of electron density Ne of dosimetric gels, with the kinetic energy of He ion.

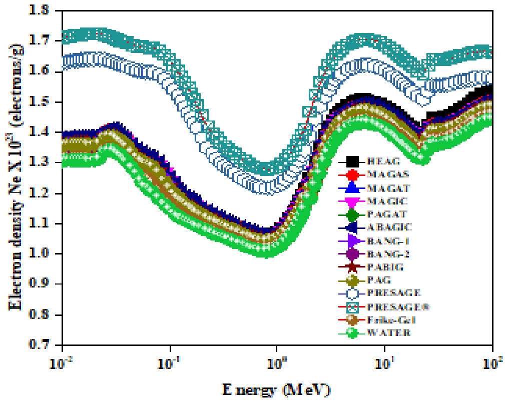

Fig. 6. Variation of electron density Ne of dosimetric gels, with the kinetic energy of B ion.

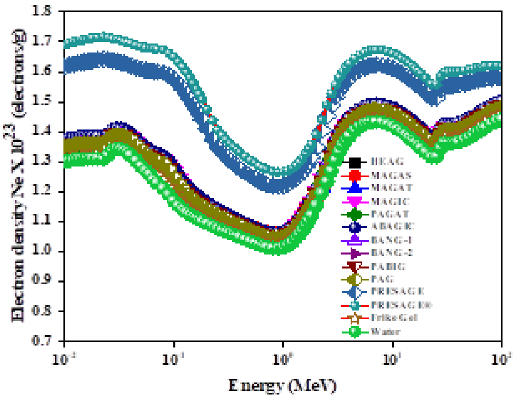

Fig. 7. Variation of electron density Ne of dosimetric gels, with the kinetic energy of C ion.

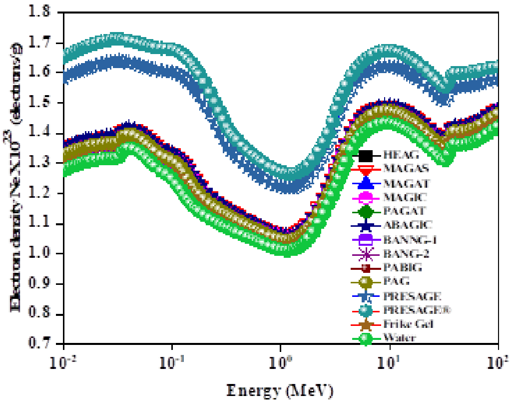

Fig. 8. Variation of electron density Ne of dosimetric gels, with the kinetic energy of O ion.

Table 1. Statistical information on Z_{eff} of the Gel dosimeters for He, B, C, and O ions. (1) HEAG (2) MAGAS (3) MAGAT (4) MAGIC (5) PAGAT (6) ABAGIC (7) BANG-1 (8) BANG-2 (9) PABIG (10) PAG (11) PRESAGE (12) PRESAGE® (13) Fricke Gel (14) Water.

S. N	He ion				B ion				C ion				O ion			
	Mean	STD	Min	Max	Mean	STD	Min	Max	Mean	STD	Min	Max	Mean	STD	Min	Max
1	3.00	0.21	2.65	3.27	3.03	0.34	2.44	3.47	3.03	0.33	2.44	3.47	3.03	0.32	2.45	3.44
2	3.04	0.21	2.67	3.30	3.06	0.34	2.47	3.50	3.06	0.33	2.47	3.50	3.06	0.32	2.47	3.47
3	3.04	0.21	2.67	3.30	3.06	0.33	2.47	3.50	3.06	0.33	2.47	3.49	3.06	0.32	2.48	3.47
4	3.04	0.21	2.67	3.31	3.07	0.34	2.47	3.51	3.07	0.33	2.47	3.50	3.06	0.32	2.47	3.47
5	3.01	0.21	2.66	3.28	3.04	0.34	2.45	3.48	3.03	0.33	2.44	3.46	3.03	0.32	2.45	3.45
6	3.04	0.21	2.67	3.30	3.06	0.34	2.46	3.50	3.06	0.33	2.47	3.49	3.06	0.32	2.47	3.47
7	3.00	0.21	2.65	3.27	3.03	0.34	2.44	3.47	3.03	0.33	2.44	3.47	3.03	0.32	2.44	3.45
8	3.02	0.21	2.66	3.29	3.04	0.34	2.45	3.49	3.04	0.34	2.45	3.49	3.04	0.33	2.46	3.46
9	3.02	0.21	2.66	3.29	3.05	0.34	2.45	3.49	3.05	0.33	2.46	3.49	3.04	0.32	2.46	3.46
10	3.01	0.21	2.65	3.28	3.04	0.34	2.44	3.48	3.04	0.33	2.45	3.47	3.03	0.32	2.45	3.45
11	3.27	0.20	2.88	3.51	3.32	0.31	2.70	3.64	3.32	0.31	2.70	3.63	3.32	0.31	2.70	3.63
12	3.24	0.19	2.87	3.52	3.35	0.32	2.72	3.67	3.31	0.31	2.69	3.65	3.31	0.31	2.69	3.64
13	2.99	0.25	2.52	3.30	3.03	0.34	2.44	3.51	3.03	0.34	2.44	3.50	3.02	0.33	2.45	3.46
14	2.93	0.24	2.47	3.22	2.98	0.34	2.40	3.44	2.98	0.34	2.40	3.43	2.97	0.32	2.41	3.41

The Z_{eff} variation for He ion is up to 21%, 25%, and 20% for hypoxic and normoxic gels, Fricke gel, and PRESAGE gels, respectively. For other ions, variation is up to 34% for hypoxic and normoxic gels, Fricke gel, and 32% for PRESAGE gels. Generally, as shown in Fig.1 to Fig.8, Z_{eff} and N_e behavior with ion energy for all dosimeters studied in this work are similar high values at low energy range (10 – 100 keV) decreasing gradually with energy increasing till reaching its minimum values (0.2 MeV for He, around 0.8 MeV for B & C, and 1.2 MeV O ion), within mid-range (100 keV – 10 MeV).

Increasing again to reach maximum values at 2.75 keV, 6.5 MeV, 7 MeV, and 9 MeV for He, B, C, and O ion, respectively, and then it decreases to a minimum at 8, 22.5, 25, and 32.5 MeV. Another sharp increase to 10, 27.5, 30, and 40 MeV for He, B, C, and O ion occurs then decreases steadily till the end of the energy range. The exception is for PRESAGE and PRESAGE® that have maximum values at low energy and high values at mid energies. Higher values for Z_{eff} are observed in PRESAGE and PRESAGE® for all types of ions whereas the lowest values are observed in water. The peaks of Z_{eff} values are shifted toward higher energies with the increase of incident ion Z number as shown for some selected gels in Fig. 9 to Fig 12 below.

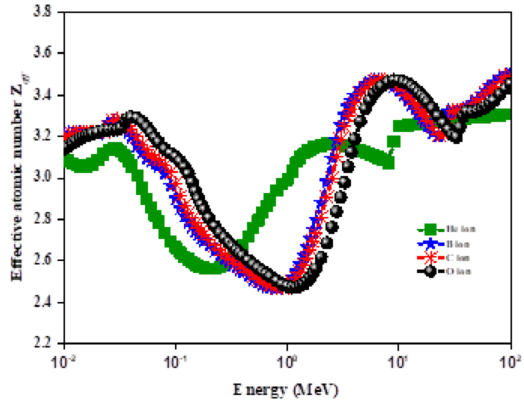

Fig. 9. Zeff of selected gel dosimeters for different types of ions in MAGIC gel.

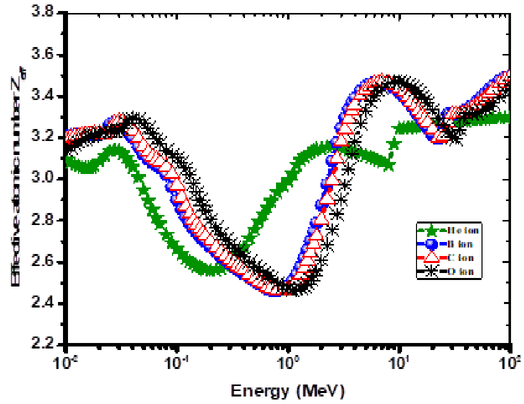

Fig. 10. Zeff of selected gel dosimeters for different types of ions in ABAGIC gel.

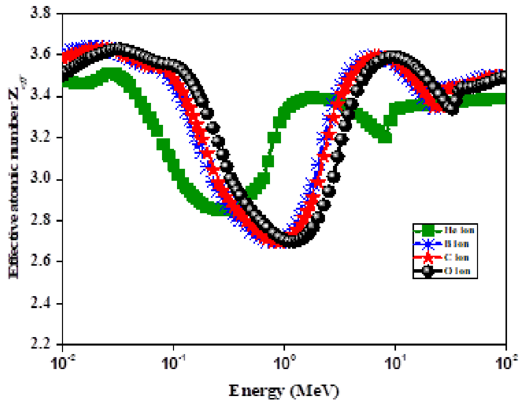

Fig. 11. Zeff of selected gel dosimeters for different types of ions in PRESAGE.

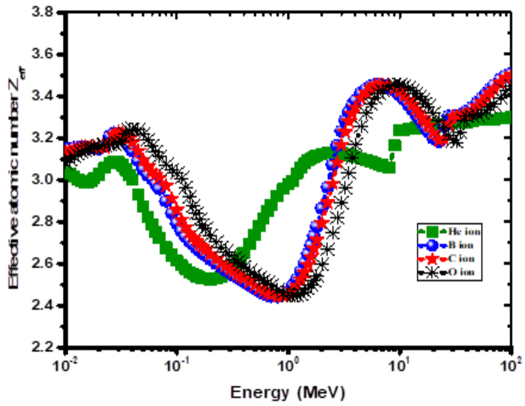

Fig. 12. Zeff of selected gel dosimeters for different types of ions in Fricke gel.

A convenient method for evaluating the radiological characteristic equivalence of two materials is to compare Z_{eff} and N_e in a continuous energy region. Therefore, Z_{eff}s of the materials relative to water were also calculated to show the water equivalence of each material. It is found that Z_{eff} values of polymeric gels and Fricke gel and their behavior concerning ion energy are very close to those of water. Fig.13 to Fig.16 below shows the percentage difference of <7% for all types of incident ion. These gels could be considered as water equivalent material throughout the entire range of energy studied. PRESAGE gels show differences of up to 17.5%, 22%, 21%, and 25% for He, B, C, and O ion, respectively. It is worth saying that PRESAGE and PRESAGE® show differences of 5% in the energy range 10 – 100 MeV of He ion. The highest differences for all gels studied occur between 40 and 300 keV energies for all ions.

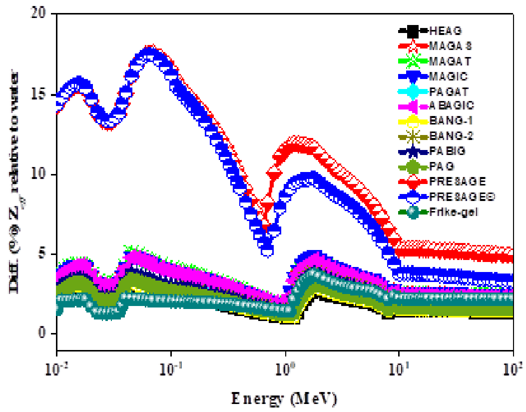

Fig. 13. Percentage difference in Zeff of gel dosimeters relative to water for He ion interaction.

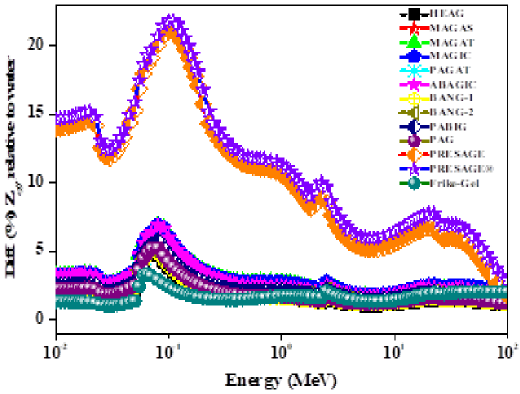

Fig. 14. Percentage difference in Zeff of gel dosimeters relative to water for B ion interaction.

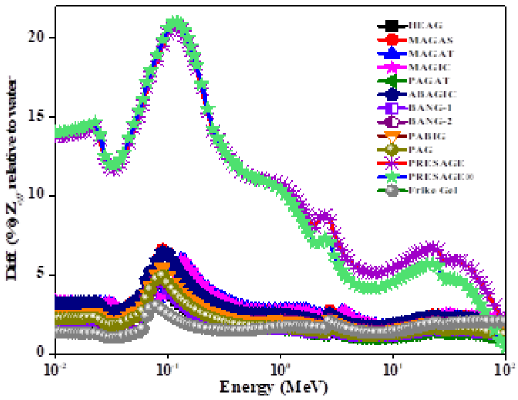

Fig. 15. Percentage difference in Zeff of gel dosimeters relative to water for C ion interaction.

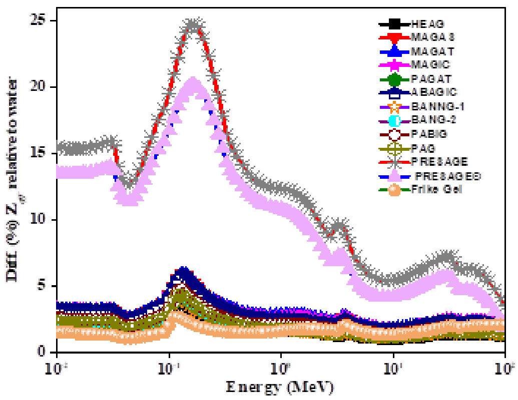

Fig. 16. Percentage difference in Zeff of gel dosimeters relative to water for O ion interaction.

Fig. 5 to Fig.8 shows the variation of electron density of up to 10%, 14%, 15%, and 14% for He, B, C, and O ion, respectively, with ion energy. This variation shows the same behavior as Z_{eff} toward incident ion energy for all types of ions, which is expected since the values of N_e depends mainly on Z_{eff}. No experimental data were available concerning Z_{eff} and N_e for gels under study. There are only a few data of calculated Z_{eff} and N_e for PRESAGE, MAGAT, MAGIC, and Fricke gel interaction with He, B, and C ion in the limited energy range 0.01–10 MeV [9]. A good agreement is achieved in comparison.

4. Conclusion

In the present study, Z_{eff} and N_e of water, Fricke gel, and 10 polymeric gel dosimeters were calculated for He, B, C, and O ion interaction in the energy range 10 keV–100 MeV. We have shown that variation in Z_{eff} values is observed in the entire energy region from 10 keV to 100MeV. The lowest values of Z_{eff} were obtained in water, whereas the highest values were obtained in PRESAGE and PRESAGE®. These high values are due to the presence of a high Z element (Br, Z = 35) with a relatively high weight fraction within its constituents. The maximum values of Z_{eff} depend on ion type and shift toward higher energies with increasing the atomic number of the incident ion.

All polymeric gels and Fricke gel investigated found to be water-equivalent materials within the entire energy range studied. Further studies for different PRESAGE formulations regarding their water and tissue equivalence and other radiological properties are necessary when using them for dose measurements. Electron density is closely related to the effective atomic number and has the same quantitative energy dependence as $Z_{eff.}$ Data reported here gives essential information about the interaction of different types of charged particles with different materials and could be useful in the energy range specified.

References

[1] R. C. Murty, Nature **207**(4995), 398 (1965).
[2] C. Baldock, IOP Publishing **777**(1), 012029 (2017).
[3] M. L. Taylor, R. D. Franich, J. V. Trapp, P. N. Johnston, Australasian Physics & Engineering Sciences in Medicine **31**(2), 131 (2008).
[4] M. L. Taylor, R. D. Franich, J. V. Trapp, P. N. Johnston, Radiation research **171**(1), 123 (2009).
[5] M. Kurudirek, Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms **336**, 130 (2014).
[6] M. Kurudirek, T. Onaran, Radiation Physics and Chemistry **112**, 125 (2015).
[7] M. Kurudirek, Applied radiation and Isotopes **94**, 1 (2014).
[8] M. Kurudirek, Radiation Physics and Chemistry **102**, 139 (2014).
[9] M. Kurudirek, Detectors and Associated Equipment **795**, 239 (2015).
[10] M. Kurudirek, O. Aksakal, T. Akkuş, Radiation and environmental biophysics **54**(4), 481 (2015).
[11] M. Kurudirek, International Journal of Radiation Biology **92**(9), 508 (2016).
[12] M. Büyükyildiz, The European Physical Journal Plus **132**(9), 391 (2017).
[13] S. Brown, A. Venning, Y. De Deene, P. Vial, L. Oliver, J. Adamovics, C. Baldock, Applied Radiation and Isotopes **66**(12), 1970 (2008).
[14] T. Gorjiara, Z. Kuncic, S. Doran, J. Adamovics, C. Baldock, Medical physics **39**(11), 7071 (2012).
[15] J. F. Ziegler, M. D. Ziegler, J. P. Biersack, Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms **268**(11-12), 1818 (2010).

[16] J. F. Ziegler, M. D. Ziegler, J. P. Biersack, SRIM (http://www. srim. org/), 12 (2014).

[17] M. H. Eisa, A. H. A. Alfedeel, Digest Journal of Nanomaterials and Biostructures, **15**(1), 59(2020)

[18] D. F. Jackson, D. J. Hawkes, Physics Reports **70** (3), 169 (1981).