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SECTION 3. Nanotechnology. Physics.

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WAKE EFFECTS INDUCED IN LIQUID WATER BY HYDROGEN-**DICLUSTER IONS**

Abstract: A theoretical model has been established to simulate the penetration process of hydrogen dicluster ions targeting liquid water at five incident energies [0.05, 0.25, 0.1, 0.2 and 2.5] MeV. This study is a novel approach in management the induced spatial potential related to the stochastic nature of energy loss in matter of single and correlated proton of hydrogen-dicluster beam radiation on H2O, aiming to explore the effects of the induced wake potential by hydrogen dicluster ions on the liquid water, H2O. This study was conducted in department of physics/ college of science, Al-Mustansiriya University in Iraq. The induced spatial potential by the incident diclusters is described by the dielectric response formalism, in which the Drude dielectric function and plasmon-pole approximation, PPA are adopted to provide a detailed evaluation to the studied wake potential [1, 2]. Calculations have been done for each elements of H2O, then apply Bragg's rule [3]. In the case of singleproton of hydrogen dicluster ions (denoted as uncorrelated ions), the wake potential is nearly independent of incident energy of H2+-dicluster ions. It is found that the dynamical interaction potential between dicluster ions leads to a spatial asymmetry to the cluster structure.

Key words: Wake potential, Hydrogen-dicluster ion, liquid water. Language: English

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Introduction

Since the discovery of radiation, the interaction of ionizing radiation with living tissues has become of prime interest in many branches such as: medical oncology, radiation protection physics, and astrophysics. The interaction of energetic charged particles with biological medium is primarily through coulomb forces resulting in losing energy to their environment by ionizations and excitations of the atoms and molecules within the cell, secondary electrons and radicals are formed thus; further ionizations are induced near the primary path of the particle.

Liquid water is present in all living matter (70-80% in soft tissue) [4], Most of the living tissue of a human being is made up of water; it constitutes about 92% of blood plasma, about 80% of muscle tissue, about 60% of red blood cells, and over half of most other tissues.

When ionizing radiation passes through living tissue, electrons are removed from neutral water molecules to produce H₂⁺O ions, the radicals formed

when ionizing radiation passes through water are among the strongest oxidizing agents that can exist in aqueous solution.

One of the significant processes that take place between the cluster ions and the target interactions is the induced wake potential, the dielectric formulation that deals with such studies that describes the way these interactions take place in which it is specified in terms of the induced wake potential gives the response of the medium to the perturbation created by the moving cluster ion [5-7]. The passage of a cluster projectile through a target generates an electric potential where the coulomb field of the moving cluster ions polarizes the electron density around the projectile path in the target causing the dissociations of the electrons from their equilibrium positions [8]. In clusters, the electric potential gives rise to further disturbance in the transport of electrons produced by other cluster ions [9].

In current study, a detailed calculation of the induced wake have been made particular in the dynamical interactions among hydrogen dicluster correlated and self-ions moving in the H₂O in



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incident energy range (0.05, 0.25, 1.0, 2.0, and 2.5) MeV, taking in consideration the damping using the random phase approximation, RPA dielectric function to represent the response of the biological medium.

Wake Potential of Swift Hydrogen-Dicluster Ions

Electronic excitations will be induced by an energetic swift hydrogen dicluster ions passing through H₂O, an accompanying wake potential ($Ø_{ind.}$) will appear in the neighborhood of the external H₂⁺⁻

ion as it passes through the stopping medium. As a result, a retarding force acts on the H_2^+ - dicluster ion and causes it to lose energy.

Since the induced wake potential produced by a proton of velocity \vec{U} moving through a material characterized by its dielectric properties $\in (\vec{k}, \omega)$, [using Drud's dielectric approach in the present study] is expressed as [10]:

$$\phi_{\text{ind.}} = \frac{Z_1}{2\pi} \int \frac{d^3 k}{k^2} e^{i\vec{k}.\vec{r}} \left[\frac{1}{\in (\vec{k}, \vec{k}.\vec{v})} - 1 \right]$$
(1)

Where ϕ_{ind} is the induced potential, \vec{r} is the vector measured from the instantaneous of the proton.

To redefine the wake potential for hydrogen dicluster ions, one can start from the following simple formula:

$$\phi_{ind} = -Z_i e \int \vec{E} d\vec{r}, \qquad d\vec{r} = \vec{v} dt \qquad (2)$$

Where $Z_i e$ is the charge of the stopping medium, \vec{E} is the electric field multiplied by a differential change of the distance. And since the stopping power of a dicluster is represented as the following equation [11],

$$\mathbf{S}_{clu}(q) = \mathbf{S}_{s}(q) + \mathbf{S}_{corr}(q)$$
⁽³⁾

Then insertion of Eq. (3) into Eq. (2) with $d\vec{r} = \vec{v}dt$ yields the following expression for the induced potential,

$$\phi_{\text{ind.}} = \sum_{j} \frac{2Z_{j}e}{\pi v} \sum_{i} Z_{i}e \int \frac{-\vec{k}.d\vec{k}}{k^{2}} |\rho_{q}(k)|^{2} \int d\omega \left[Cos(\vec{k}.\vec{r}_{ji}) \operatorname{Re}\left[\frac{1}{\in(\vec{k},k.v)}\right] - Sin(\vec{k}.\vec{r}_{ji}) \operatorname{Im}\left[\frac{1}{\in(\vec{k},k.v)}\right] \right]$$
(4)

Where:
$$|\vec{k}| = \frac{w}{v}$$

 $\vec{k} \cdot \vec{r_{ij}} = \frac{w}{v}r$
 $\vec{r}_{ji} = \vec{r}_j - \vec{r}_i$

From the condition of dielectric function:

$$\in (-\bar{k},-\omega) = \in^* (\bar{k},\omega).$$

The imaginary part in Eq. (4) is dissipative because:

$$Sin(-\vec{k}, \vec{r}_{ji}) = -Sin(\vec{k}, \vec{r}_{ji})$$
$$Cos(-\vec{k}, \vec{r}_{ji}) = Cos(\vec{k}, \vec{r}_{ji})$$

It is important to keep in mind that the induced potential is written in real form and the force is written in imaginary form therefore, Eq. (4) becomes,

$$\phi_{\text{ind.}} = \sum_{j} \frac{2Z_{j}e^{2}}{\pi v} \sum_{i} Z_{i} \int \frac{\vec{k}.d\vec{k}}{k^{2}} \left| \rho_{q}(k) \right|^{2} \int d\omega \left[Cos(\vec{k}.\vec{r}_{ji}) \operatorname{Re}\left[\frac{1}{\in (\vec{k},k.v)}\right] \right]$$
(5)

The next step is to drive the induced potential for H_2^+ - dicluster ions by separating the terms i = jfor self-ions and $i \neq j$ for correlated ions of the inter-

nuclear separation \vec{r}_{ji} and by summing up them together we get,



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$$\phi_{ind} = \frac{2e^2}{\pi v} \int_0^\infty \frac{d\vec{k}}{\vec{k}} |\rho_q(k)|^2 \int_0^{\vec{k}.\vec{v}} d\omega \operatorname{Re}\left[\frac{1}{\in (\vec{k},\vec{k}.\vec{v})}\right] \left[\sum_i z_i^2 + \sum_{i\neq j} z_i z_j \operatorname{Cos}(\vec{k}.\vec{r}_{ji})\right]$$
(6)
$$= \phi_{self} + \phi_{correlated}$$

Where,

$$\phi_{self} = \frac{2e^2}{\pi v} \int_0^\infty \frac{d\vec{k}}{\vec{k}} \left| \rho_q(k) \right|^2 \int_0^{\vec{k}.\vec{v}} d\omega \operatorname{Re}\left[\frac{1}{\in (\vec{k},\vec{k}.\vec{v})}\right] \sum_i z_i^2 \tag{6} a$$

$$\phi_{corr.} = \frac{2e^2}{\pi v} \int_0^\infty \frac{d\vec{k}}{\vec{k}} \left| \rho_q(k) \right|^2 \int_0^{\vec{k}.\vec{v}} d\omega \operatorname{Re}\left[\frac{1}{\in (\vec{k},\vec{k}.\vec{v})}\right] \left[\sum_{i \neq j} z_i z_j \operatorname{Cos}(\vec{k}.\vec{r}_{ji}) \right]$$
(6) b

Where $\rho_q(k)$ the Fourier is transform of the projectile charge density $\rho_q(r)$ for the charge state q and is given in the following equation,

$$o(q) = \frac{q + (k\Lambda)^2}{(k\Lambda)^2} \tag{7}$$

JIF

In present work we will calculate the self and correlated wake potential for each element in H₂O then applying Bragg's rule to the correlated. A computer program "Zanb-cluster. For" has been written for numerical calculations liquid water [12]

Results and Discussion

Results will be summarized and presented as figures; we shall try to demonstrate the effects of wake potential on H₂O following the dielectric formalism, calculations has been made for wake potential produced by a moving H₂⁺-dicluster ions

through H₂O target. The wake potential for single and correlated ions has been calculated using Eq. (6). These calculations were made without comparing with experimental data because of the lack in such data for H₂O target.

Figure (1) represents the variation of induced wake potential for self-interaction Φ_s , with charge exchange, q in liquid water. For liquid water, at $q \rightarrow$ 1 where H2+-dicluster ions are fully ionized, the maximum differences between the values of selfwake potential is about ≈ 10 %. Also, it has been noted in H_2O that at q = 0 the wake potential was $\Phi_{\rm s} = 0.0038$ a.u.

This difference in Φ_s of H₂O is probably due to combination of its structure and the collective effect (vicinage effect) between H₂⁺-dicluster ions in one hand and with the target material in another hand Fiq.1.

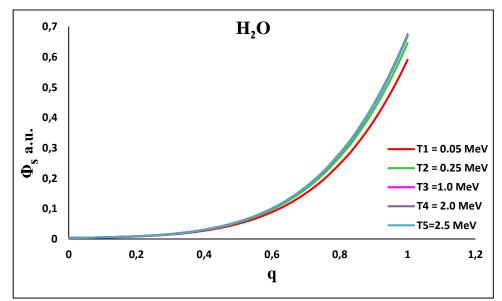


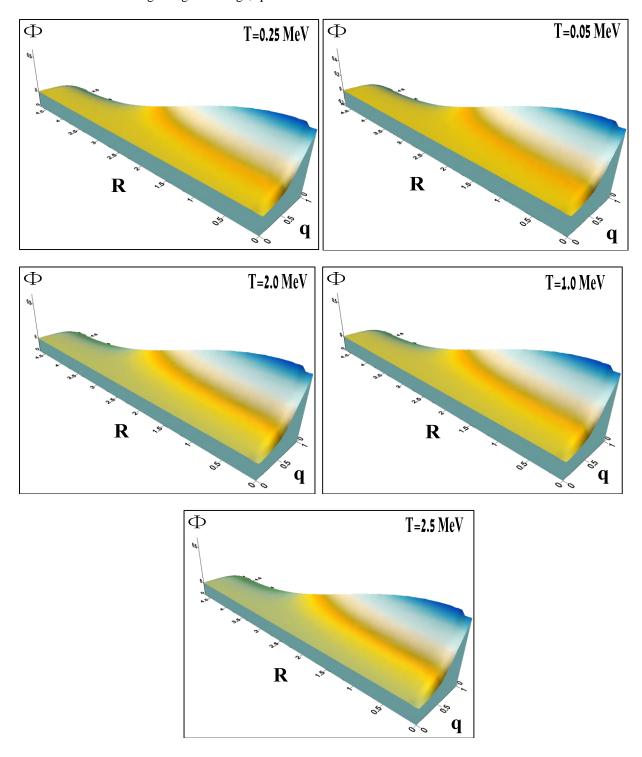
Figure 1 - Self-Induced wake potential, Φ_s versus charge fraction, q, at five different incident H₂⁺- dicluster ions energies (0.05, 0.25, 1.0 2.0, 2.5) MeV for H₂O.



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It is seen very clearly from Fig. (2) that the correlated potential of H₂O is affected by the charge fraction q, and the inter-nuclear distance R, at five incident energies of H₂⁺-dicluster ions T_i (0.05,0.25, 0.1, 0.2, and 2.5) MeV. At R \rightarrow 0, the wake potential increases with increasing charge exchange, q until it

reaches its maximum, while at $R \rightarrow \infty$, the wake potential becomes independent of q as shown in figure below. The $\Phi_{corr.}^{H_2O}$ spectrum was decreasing as R increased dropping to the lowest value at $R \sim 3$.



 $\label{eq:Figure 2-Induced wake potential Φ_c for correlated interaction versus charge fraction, q, at five different incidents H_2^+- dicluster ions energies (0.05, 0.25, 1.0, 2.0 and 2.5) MeV for H_2O.}$



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Conclusion

The results of current study reveal that both self and correlated hydrogen dicluster ions produce spatial ionizations and excitations of electrons along their penetration path inside the target H₂O spatially at the Bragg region. It is seen from results throughout the whole work that the correlated term of H₂⁺ dicluster ions is strongly influenced by the internuclear distance R, and with charge exchange q.

From the point of view of cluster-atom collisions and by using the results of this study, the spatial collective effects of the induced wake potential and the other important physical processes resulted after H_2^+ -dicluster ions- H_2O interaction, such as energy loss, energy loss straggling, charge exchange and other processes, it is expected that the initial structures of both the hydrogen dicluster ions and the H_2O is to be rearranged thus, leading to the changing in their characteristics which agrees with the work of Garcia et.al 2005 [13].

Since water makes up most of the cell's volume (about 70 %) Therefore, the probability of radiation beam interacting with the cellular water is much higher thus producing free radical and active oxygen species that follows a cascade of events [14]. At the molecular level, these oxidizing agents destroy critical biological targets such as DNA by either removing electrons or removing hydrogen atoms which often leads to base damge BD, single-strand breaks SSB and double- strand breaks DSB of DNA [12, 15].

The results of this study reveals that at malignant cells, the DNA environment will be modified after irradiation with H_2^+ -dicluster ions by neutralizing the free radicals that exits at the same tumor cells, thus, these cells eventually will be killed and as a general result a cure from cancer disease is obtained in a quick and conformable way without needing to surgical interference.

The effects of water radicals are responsible for about 65 % of cellular DNA damage, while the direct effects contribution are about 45 % [16].

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