SECTION 3. Nanotechnology. Physics.

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 single-proton 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 physics, oncology, radiation protection 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 H$_2^+$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 H$_2$O in...
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 H$_2$O, an accompanying wake potential ($\phi_{\text{ind}}$) will appear in the neighborhood of the external H$_2^+$-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 $\vec{v}$ moving through a material characterized by its dielectric properties $\epsilon(\vec{k}, \omega)$, [using Drud’s dielectric approach in the present study] is expressed as [10]:

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

(1)

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

$$\phi_{\text{ind}} = -Z_i e \int \vec{E} \cdot d\vec{r}, \quad d\vec{r} = \vec{v}dt$$

(2)

Where $Z$, $e$ 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],

$$\phi_{\text{ind}} = \sum_i \frac{2Z_i e}{\pi \nu} \sum_j Z_j e \left[ \frac{-\vec{k} \cdot d\vec{k}}{k^2} \rho_j(k) \right]^2 \int d\omega \left[ \cos(k \cdot \vec{r}_j) \Re \left[ \frac{1}{\epsilon(k, k \cdot v)} \right] - \sin(k \cdot \vec{r}_j) \Im \left[ \frac{1}{\epsilon(k, k \cdot v)} \right] \right]$$

(3)

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

$$S_{\text{du}}(q) = S_s(q) + S_{\text{corr}}(q)$$

(4)

$$\sin(-\vec{k}, \vec{r}_j) = -\sin(\vec{k}, \vec{r}_j)$$

$$\cos(-\vec{k}, \vec{r}_j) = \cos(\vec{k}, \vec{r}_j)$$

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,

$$\phi_{\text{ind}} = \sum_j 2Z_i e^2 \sum_i Z_j e \left[ \frac{-\vec{k} \cdot d\vec{k}}{k^2} \rho_j(k) \right]^2 \int d\omega \left[ \cos(k \cdot \vec{r}_j) \Re \left[ \frac{1}{\epsilon(k, k \cdot v)} \right] \right]$$

(5)

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

$$\phi_{\text{ind}} = \sum_j 2Z_i e^2 \sum_i Z_j e \left[ \frac{-\vec{k} \cdot d\vec{k}}{k^2} \rho_j(k) \right]^2 \int d\omega \left[ \cos(k \cdot \vec{r}_j) \Re \left[ \frac{1}{\epsilon(k, k \cdot v)} \right] \right]$$

The next step is to drive the induced potential for H$_2^+$-dicluster ions by separating the terms $i = j$ for self-ions and $i \neq j$ for correlated ions of the inter-
\[
\phi_{\text{ind}} = \frac{2e^2}{\pi v} \int_0^\infty \frac{dk}{k} \left| \rho_q(k) \right|^2 \int_0^{k,\nu} d\omega \Re \left\{ \frac{1}{\ell (k, k, \nu)} \left[ \sum_{i \neq j} z_i^2 + \sum_{i \neq j} z_i z_j \cos(k \cdot \hat{r}_{ji}) \right] \right\} 
\]

(6)

\[
= \phi_{\text{self}} + \phi_{\text{corr.}}
\]

Where,

\[
\phi_{\text{self}} = \frac{2e^2}{\pi v} \int_0^\infty \frac{dk}{k} \left| \rho_q(k) \right|^2 \int_0^{k,\nu} d\omega \Re \left\{ \frac{1}{\ell (k, k, \nu)} \right\} \sum_{i} z_i^2 
\]

(6a)

\[
\phi_{\text{corr.}} = \frac{2e^2}{\pi v} \int_0^\infty \frac{dk}{k} \left| \rho_q(k) \right|^2 \int_0^{k,\nu} d\omega \Re \left\{ \frac{1}{\ell (k, k, \nu)} \right\} \sum_{i \neq j} z_i z_j \cos(k \cdot \hat{r}_{ji}) 
\]

(6b)

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,

\[
\rho(q) = \frac{q + (\hbar k)^2}{(\hbar k)^4} 
\]

(7)

In present work we will calculate the self and correlated wake potential for each element in \( H_2O \) 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 \( H_2O \) following the dielectric formalism, calculations has been made for wake potential produced by a moving \( H_2^+ \)-dicluster ions through \( H_2O \) 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 \( H_2O \) target.

Figure (1) represents the variation of induced wake potential for self-interaction \( \Phi_s \), with charge exchange, \( q \) in liquid water. For liquid water, at \( q \rightarrow 1 \) where \( H_2^+ \)-dicluster ions are fully ionized, the maximum differences between the values of self-wake potential is about \( \approx 10 \% \). Also, it has been noted in \( H_2O \) that at \( q = 0 \) the wake potential was \( \Phi_s = 0.0038 \) a.u.

This difference in \( \Phi_s \) of \( H_2O \) is probably due to combination of its structure and the collective effect (vicinage effect) between \( H_2^+ \)-dicluster ions in one hand and with the target material in another hand Fig.1.

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**Figure 1** - Self-Induced wake potential, \( \Phi_s \) versus charge fraction, \( q \), at five different incident \( H_2^+ \)-dicluster ions energies (0.05, 0.25, 1.0, 2.0, 2.5) MeV for \( H_2O \).
It is seen very clearly from Fig. (2) that the correlated potential of H$_2$O is affected by the charge fraction q, and the inter-nuclear distance R, at five incident energies of H$_2^+$-dicluster ions T$_i$(0.05, 0.25, 0.1, 0.2, and 2.5) MeV. At R → 0, the wake potential increases with increasing charge exchange, q until it reaches its maximum, while at R → ∞, 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 ~ 3.

![Diagram of induced wake potential for H$_2$O](image)

Figure 2 - Induced wake potential $\Phi_r$ 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$_2$O.
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 inter-nuclear 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 H₂⁺-dicluster- H₂O 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 H₂O 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 damage 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 H₂⁺-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 inference.

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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