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Interference function effect when dicluster hydrogen ion interaction with solid matter with no damping

Saher Mazeher Matesher
Thi-Qar University, collage of medicine

Abstract:

This research discuss interaction of dicluster hydrogen ions with solid matter with no damping. its study traveling dicluster through solid targets (Se,Ag,Ge,Cs). we canvas interference function (vicinage function) of dicluster hydrogen ions at high and low velocities and we study the effect of wigner-seitz radius (density parameter r_s) on vicinage function (interference function) under different adverb. this research give detailed studying about interference effect of dicluster hydrogen ions at its traveling through solid matter .

1. Introduction :

In the velocity range where the energy loss of charged particles in the matter is dominated by the electronic stopping power regime, the energy loss per ion in solids is known to be significantly different for molecular projectiles, as compared with independent ions at the same velocity [1] This difference has been interpreted as originated from the so called *vicinage effect,* which can be obtained either from a dielectric or atomic description of the energy loss in solids [2]. The vicinage effect was theoretically explained as a result of the excitation of target electrons by the simultaneous interactions of two or more ions moving in a correlated way at short inter ion distances through the solid. It was also demonstrated that this interference effect could be constructive or destructive, according to the velocity of the molecular projectile and the inter ion distance. When the molecule enters the solid, the ions from the cluster will lose their electrons in the first few atomic layers of the target, remaining as an aggregate of positively

charged ions. Then, due to the Coulomb repulsion, the molecule will explode, the ions begin to separate, and the interference effect will start to smear out, disappearing after a certain characteristic distance. The vicinage effects depend on the molecular geometry and velocity as well as on the properties of the stopping medium.[3]

2. Stopping power

2-1 Slowing down of charged particles in materials

An energetic ion (projectile) penetrating in a medium interacts with the target atoms. It collides with the nuclei and electrons of the target, the interactions lead to a loss of the ion's energy. In the energy range of 0-10^4eV/amu, the energy loss per unit length per atom i.e. the stopping power, can be divided into nuclear stopping and electronic stopping terms[4]. The nuclear stopping governs the energy losses caused by elastic collisions between the ion and the nuclei of atoms in the target. The electronic stopping terms governs the energy losses caused by the electronic interactions, which can be further divided into several different contributions depending on the nature of the interaction. Hence, the stopping power can be written as [5].

$$\frac{dE}{dx}=\left(\frac{dE}{dx}\right)_{nuclear}+\left(\frac{dE}{dx}\right)_{electrons} \qquad ...(1)$$

For high energies, contributions coming from nuclear reactions and relativistic corrections have to be taken into account. However, they can be neglected in the context of this project as the particle velocities are far below the velocity of light. There are some experimental and theoretical works [5,6] shows that the nuclear stopping term of an atom in a cluster is less than nuclear stopping power of a single charged particle (ions)[7] .

2-2 Nuclear stopping

The nuclear stopping is a sum of the energy losses of a moving ion due to its elastic collisions with the target nuclei. The energy that an ion losses is converted to heat in the slowing down material as the atoms spread the kinetic energy in series

collisions, namely in collision cascades. A common feature for all ions is that the nuclear stopping as a function of ion energy has a maximum at a relatively low energy and that the nuclear stopping of the ion decreases as the energy of the ion increases[8]. This means that the nuclear stopping is important only for a very low ion velocities [7].

2-3 Electronic stopping

Electronic stopping is a common term for the energy losses caused by all electronic processes. It originates from several different contributions depending on the type of the interaction, ions moving faster than ~10^4eV/amu loss kinetic energy mainly via electronic stopping, see Fig. (1)[9].

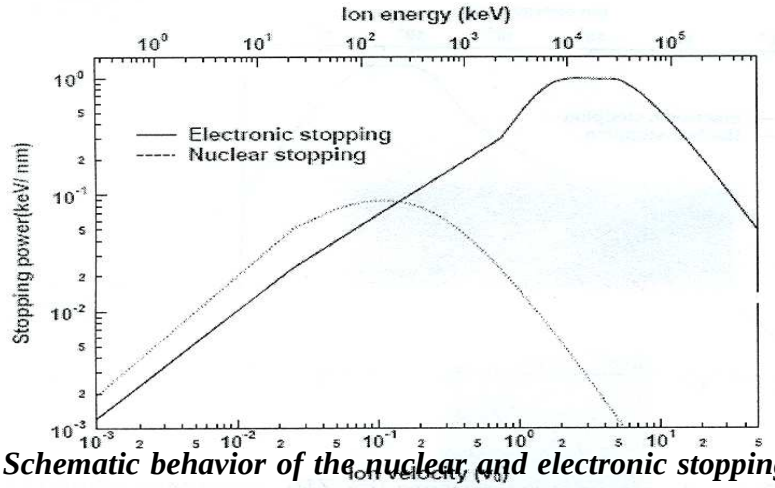

Figure (1): Schematic behavior of the nuclear and electronic stopping as a function of ion velocity [9]

When an ion moves inside the material, it collides with the electrons of the material, which can be either bound or free. In metals the electrons are divided into bound core electrons and free conductive electrons. If the ion is moving slowly, it carries all of its electrons with it. If the ion is moving faster than the fastest target electrons, it losses all its electrons and is completely ionized[6]. These cases are the theoretically best understood ones [10]. An ion moving slowly losses energy only to the free electrons of

the target due to momentum exchange with them . Due to the forbidden energy levels , this results in a linear dependence of the stopping on velocity [11]. A high velocity ion can be considered to be a point-like charge, which can collide with all electrons in the target. The stopping is then inversely proportional to the square of the ion velocity [12]. When the ion velocity is between these two cases, the ion is partially stripped leading to considerably more complicated description [13], because the ion may lose electrons to and capture them from the medium.

2-4 *Stopping power of cluster ionic* :

When swift cluster impinge on a solid their binding electrons are stripped off after traversing the first atomic layers forming then a cluster of atomic ions(14). In the context of swift cluster-beams bombarding a solid when the cluster velocity v is larger than Fermi velocity v_F, it loses energy due mainly to the interaction with target electrons. Then, in what follow we will consider only the electronic stopping power of swift cluster in solid, neglecting the contribution of nuclear stopping power . The electronic stopping power of a swift charge moving inside is satisfactorily well described within dielectric formalism (k,w) of the stopping medium, the stopping power of a cluster of n charge Ze moving at velocity v is then given by[3]

$$Sclu = \sum_{1}^{n} Z_{i}^{2} S_{p} + \sum_{i \neq j}^{n} Z_{i} Z_{j} I(r_{ij}) \qquad (2)$$

Where r_{ij} is the internuclear separation of two ions in the cluster. Here Sp is the energy loss per unit length of a single proton having the same velocity as the cluster and is given by

$$Sp = \frac{2}{\pi \upsilon^2} \int_0^{\infty} \frac{dk}{k} \int_0^{k\upsilon} dww \,\mathrm{Im}\left[\frac{-1}{\in (k,w)}\right] \quad \textbf{(3)}$$

The interference function I(r) given by

$$I(r_{ij}) = \frac{2}{\pi \upsilon^2} \int_0^{\infty} dk \frac{\sin kr}{k^2 r} \int_0^{k\upsilon} dww \,\mathrm{Im}\left[\frac{-1}{\in (k,w)}\right] \quad \textbf{(4)}$$

Describes the spatial correlation among the ions in the cluster. It becomes equal to Sp as $r_{ij} \to 0$ (the united-ion case) and goes to zero as $r_{ij} \to \infty$.

3. Calculation & results:

Consider a pair of ions z_1, z_2 in correlated motion a structure that may be obtained by the incidence of diatomic molecules with velocity $(\vec{v})$ in a dense medium of valence electrons of solid.

The main electron gas parameters to be used here are the following: Fermi velocity $(\vec{v}_F)$, plasma frequency (ω_p), and Wigner-Seitz radius of the average volume occupied by each electron in units of Bohr radius $a_o = \eta^2 / me^2 = 0.529 A^o$. (with relations: $\vec{v}_F$ = 1.919/r_s, $\omega_p = \sqrt{3/r_s^3}$ in atomic units).

i. *Low velocities* $\vec{v} < \vec{v}_F$:

The well-known Lindhard function [15] gives in a self-consistent way an exact description of the dielectric function for a non-relativistic free electron gas of high density at zero temperature. In the low frequency limit, within this Random Phase Approximation (RPA) for the dielectric function, the loss function can be written as:

$$\left.\begin{aligned} &\in(\vec{k},\omega) \cong \in_1(\vec{k}) + i \in_2(\vec{k},\omega) \\ &or \\ &\frac{1}{\in(\vec{k},\omega)} \cong \frac{1}{\in_1(\vec{k}) + i \in_2(\vec{k},\omega)} \end{aligned}\right\} \quad (5)$$

We can write the imaginary part of the dielectric function as the following [16].

$$\mathrm{Im}\left(\frac{-1}{\in(\vec{k},\omega)}\right) = \frac{\frac{4\vec{k}_F}{\pi k^2} \times \frac{\pi\omega}{2k.k_F}}{\left\{\left(\frac{4\vec{k}_F}{\pi k^2}\right)\left[\frac{1}{2}\left(1 + \frac{4k_F^2 - k^2}{4k.k_F}\ln\left|\frac{k + 2k_F}{k - 2k_F}\right|\right)\right] + 1\right\}^2 + \left[\frac{4\vec{k}_F}{\pi k^2} \times \frac{\pi\omega}{2k.k_F}\right]^2} \quad (6)$$

Thus we can write eq. 4 as the following :

$$I(r_{ij}) = \frac{2}{\pi v^2}\int_0^{\infty} dk \frac{\sin kr}{k^2 r}\int_0^{kv} dw w \frac{\frac{4\vec{k}_F}{\pi k^2} \times \frac{\pi\omega}{2k.k_F}}{\left\{\left(\frac{4\vec{k}_F}{\pi k^2}\right)\left[\frac{1}{2}\left(1 + \frac{4k_F^2 - k^2}{4k.k_F}\ln\left|\frac{k + 2k_F}{k - 2k_F}\right|\right)\right] + 1\right\}^2 + \left[\frac{4\vec{k}_F}{\pi k^2} \times \frac{\pi\omega}{2k.k_F}\right]^2} \quad (7)$$

By programming this equation where fig (1) show the interference function versus internuclear distance (r_{12}) when v=0.1 for (Se,Ag,Ge,Cs) targets while the fig (2) when v=1.00 . we note there are difference clear in behavior of (Cs) with three other targets which don't change much at change the velocities while the value of other targets become less with increasing the velocities. And we note when increasing the value of (r_{12}) the value of interference function become constant.

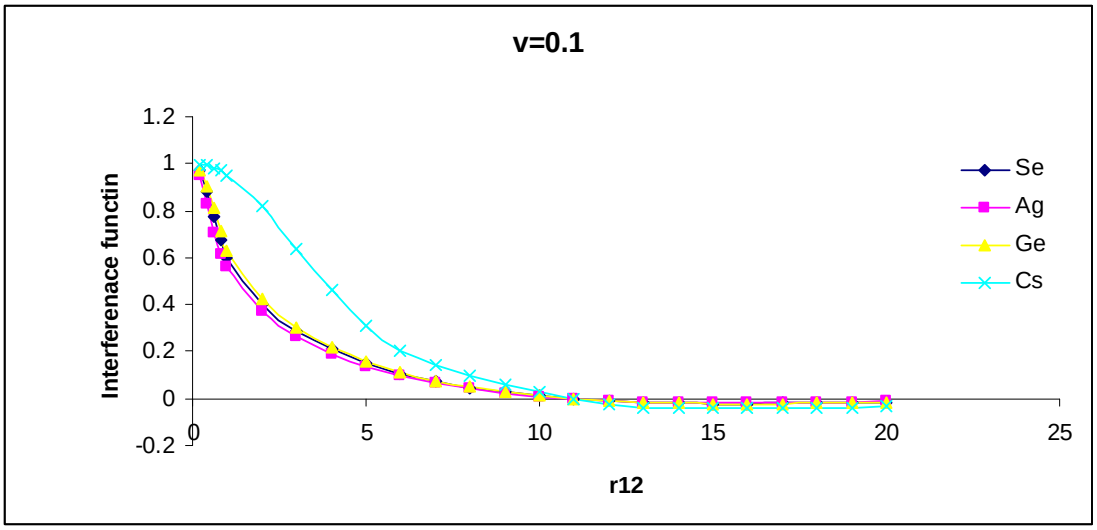

Fig.(1)the interference function of dicluster with (Se,Ag.Ge,Cs) versus internuclear distance (r_{12}) when v=0.1 .

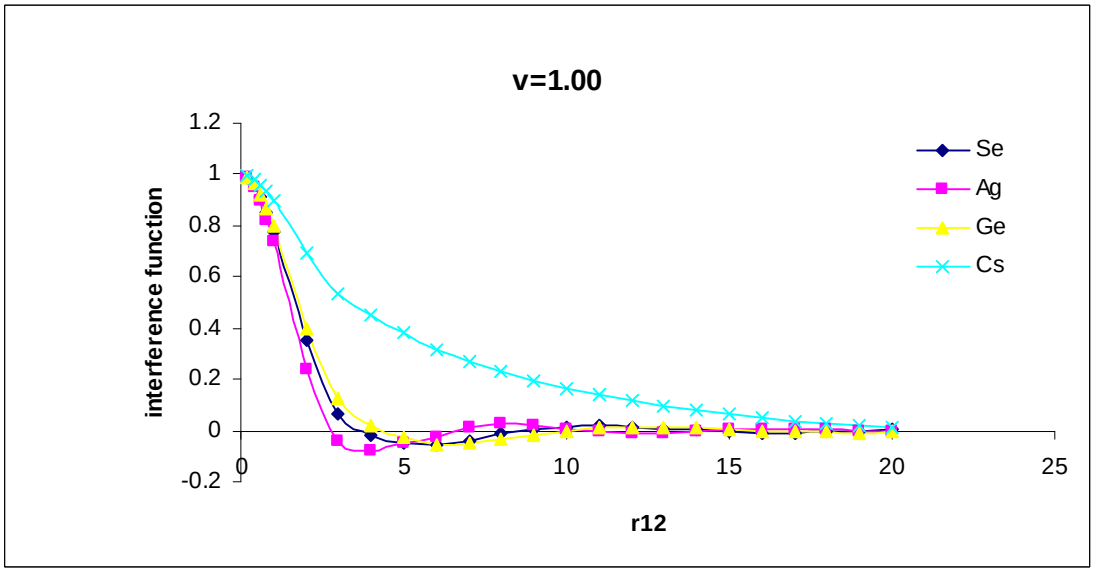

Fig.(2)the interference function of dicluster with (Se,Ag.Ge,Cs) versus internuclear distance (r_{12}) when v=1.00

ii. High velocities $v > v_F$ **:**

At high velocities, where the projectile can excite plasmons in the

medium, Brandt Kitagawa (BK) used the Plasmon Pole Approximation (PPA) of the dielectric function [16].

$$\in(\vec{k},\omega) = 1 + \frac{\omega_p^2}{\omega_g^2 + \beta^2 k^2 + \frac{k^4}{4} - \omega(\omega + i\gamma)} \qquad \textbf{(8)}$$

The plasmon frequency $\omega_p = \frac{3^{1/3}}{r_s^{3/2}}$ **and the effective band gap frequency in semiconductors and insulators give a collective resonance frequency** $\Omega_p = (\omega_p^2 + \omega_g^2)^{1/2}$ **[17]. Dispersion is included through the term containing** $\beta^2 = \frac{3}{5}k_F^2$ **where** $\vec{k}_F = 1.919 r_s^{-1}$**. Contributions from single-particle excitations are accounted for through the square of the kinetic energy** $k^2/2$ **of a free electron of momentum** $(\vec{k})$**. The small constant** γ **represents damping processes. It follows that in the limit** $\gamma \to 0$**, [16].**

$$\mathrm{Im}\left(\frac{-1}{\in(\vec{k},\omega)}\right) = \frac{\pi\omega_p^2}{2A}\delta(\omega - A) \qquad \textbf{(9)}$$

Where $A^2 = \Omega_p^2 + \beta^2 k^2 + k^4/4$

The upper and lower integration limits in $\vec{k}$ **are the maximum and minimum momentum transfers** $\vec{k}_+$ and $\vec{k}_-$ **to target electrons.**

$$\vec{k}_\pm = \left\{2(v^2 - \beta^2) \pm 2\left[(v^2 - \beta^2)^2 - \Omega_p^2\right]^{1/2}\right\}^{1/2} \qquad \textbf{(10)}$$

Which gives as threshold for $\vec{v}$**,**

$$\vec{v}_{thr.} = (\beta^2 - \Omega_p^2)^{1/2}, \qquad \textbf{(11)}$$

Then by substituting eq. (9) in eq. (4) can get :

$$I(r_{ij}) = \frac{2}{\pi \upsilon^2} \int_0^{\infty} dk \frac{\sin kr}{k^2 r} \int_0^{k\upsilon} dww \frac{\pi \omega_p^2}{2A} \delta(\omega - A) \qquad (12)$$

By using numerical method (Simson,Gausian) and After programming eq.(12) we got the following figure where fig.(3) shows the interference function for (Se,Ag,Ge,Cs) at high velocity when v= 2.00 and the fig.(4) when v=10.00 where we can note the last target (Cs) have maximum value for interference function . the interference function become constant when the value of (r_{12}) begin in increasing.

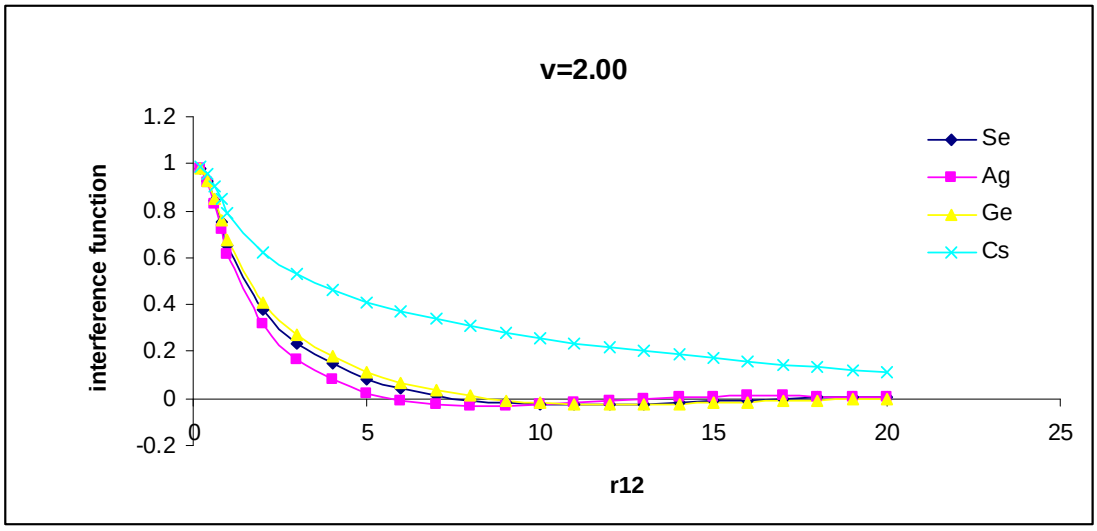

Fig.(3)the interference function of dicluster with (Se,Ag.Ge,Cs) versus internuclear distance (r_{12}) when v=2.00 .

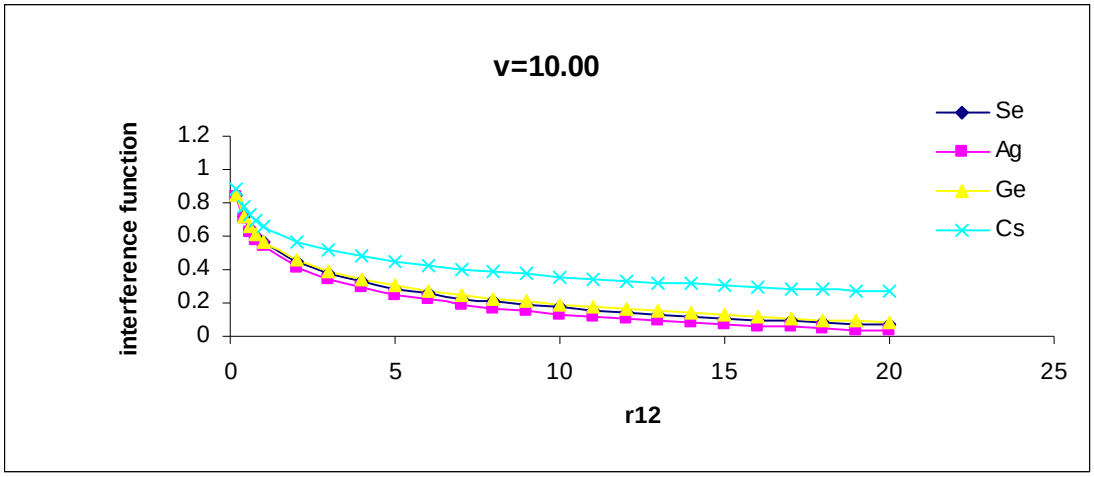

Fig.(4)the interference function of dicluster with (Se,Ag.Ge,Cs) versus internuclear distance (r_{12}) when v=10.00 .

4. Conclusion:

The stopping power, interference function, for a dicluster projectile of different internuclear distances moves at low and high velocity to interact with a piece of material of different electron densities:

$Se(r_s = 1.84)$, $Ag(r_s = 1.53)$, $Ge(r_s = 2.02)$, and $Cs(r_s = 5.88)$. **These four targets have been chosen because of their frequent use in experiments [17] also of their different electron densities, where (r_s) is a measure of electron density.**

The rise of dicluster internuclear distance decreases the value of interference function but this relation is related to the other parameters as that of electrons density, where their comparable condition ensure the maximum efficient of dicluster projectile-target interaction, as well as the effect of the dicluster velocity whither it is low to rise the aggregation influence or high velocity to stimulate the electron-hole excitation.

When dicluster internuclear distance approaches to zero to be unit atom then the vicinage effect being at the maxima value for the best performance of the two ions exchange the polarization of each one of

them. as well as that we can note the effect of the density parameter (r_s) which the (Cs) target take the maximum value while the (Ag) target have less value this because the difference of wigner seitz radius or density parameter (r_s). The increasing values of r_S leads to decrease v_F (Fermi Velocity) of a target and also the density of electrons according to the relation as $r_s = \left(\frac{3}{4\pi n_e}\right)^{1/3}$, where r_S is the radius of a sphere contains one electron [17] and *n* is the density of electrons. The impingement of dicluster in a target of small r_S means that there will be high dense of electrons to screen the projectile and retarding it. In addition, one may expect a short interaction time, therefore each target medium exhibits prevention against the projectile dependant on its density where $Ag(r_s = 1.53)$ represents the highest screening and then $Se(r_s = 1.84)$, $Ge(r_s = 2.02)$ and $C_S(r_S = 5.88)$.

At high velocities the dicluster losses its valence electrons which is regarded as interaction tool with the electron gas and this why diminishing energy exchange between fast projectile and target electrons, while at low projectile velocities, oscillating curve can be observed where the effect of charge density fluctuation when the rotating electron velocity being higher than that of a projectile to produce oscillatory Coulomb screening and so that the relation of stopping power with internuclear distance at low velocity is not linear [15].

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