MULTIPLE SCATTERING OF DEUTERIUM WAVE FUNCTION NEAR SURFACE OF PALLADIUM LATTICE

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The wave property of deuterons and the periodicity of the lattice introduce the coherences in various aspects of the interaction between the deuterons and the lattice. Multiple scattering of deuterium wave function inside a super-lattice would manifest itself through an example where the coefficients of the reflection, penetration, and absorption are calculated while a deuterium flux permeates through a palladium foil coated with alternative layers of titanium carbide and palladium. When the resonance condition is satisfied, the maximized total absorption coefficient might be greater than 50%, even if the absorption coefficient of each single layer is only less than 1%.

1. Introduction

Coherence has been an important issue to explain the abnormal phenomena in the palladium deuteride since 1989. However, the word of “COHERENCE” was used in a variety of situations such as “Q.E.D. Coherence in Matter”[1], “Ion Band State”[2], “Swimming Electron Layer Model”[3], “Selective Resonant Tunneling”[4], ……etc. If we dug into the essence of “COHERENCE”, we might find two important factors: the periodicity of the lattice and the wave nature of the deuteron. These will be the starting points of this paper.

2. Wave Nature of the Deuterons inside the Palladium Lattice

Hydrogen gas is able to permeate through the palladium foil. This property was discovered more than one hundred years ago, and it was believed that hydrogen molecule would be dissociated into hydrogen atoms first, and would be further ionized into proton and electron inside the palladium metal [5]. The proton was supposed to diffuse through the palladium foil as if proton was a granular particle. Its wave nature was usually ignored, because the diffusion model described the permeation quite well in most of the cases. Nevertheless, when the thickness of the palladium foil is less than a few microns, the permeation process is affected by the surface condition [6]. Even if the thickness is more than a few microns, the time necessary to establish the equilibrium between the hydrogen inside and outside palladium is still sensitive to the surface condition of the palladium [7]. It was familiar that a coating layer of palladium black would work like a catalyst to speed this equilibrium, but the mechanism of these anomalies are not clear. The only thing we know is that these anomalies are not explainable in terms of diffusion model. Since the discovery of the correlation between deuterium flux and heat flow in the
gas-loading phase [8, 9], we studied the dependence of the deuterium flux on the number of coating layers, and its dependence on the palladium temperature [10, 11]. Both of these dependences are not explainable in terms of diffusion model either.

2.1. Dependence on Temperature

The dependence on temperature would be quite different if different models are assumed for the permeation process. According to the diffusion model, the random walks of the deuterons are constrained by the activation energy inside the palladium lattice. When the temperature increases, more deuterons would have chance to make the random walk; hence, the diffusion coefficient is a monotonic function of the temperature. The higher the temperature, the greater the diffusion coefficient is. Consequently, the deuterium flux permeating through the palladium foil is supposed to increase with the temperature in this diffusion model. However, the experimental observation showed that there was an abnormal deuterium flux which increased while the temperature was decreasing (Fig. 1). This phenomenon appeared even if there was several coating layers on the surface of palladium surface (Fig. 2). Instead of the monotonic feature, a peak-wise feature was shown in the curves of deuterium flux versus temperature.

![Graph](image-url)

Figure 1. The solid line in the upper plot shows the deuterium flux, and the solid line in the lower plot shows the temperature of the D/Pd system. Two peaks appear clearly between 150-140°C.
Figure 2. A deuterium flux peak appears near 140°C when the temperature of D/Pd system increases. There were 3 alternative coating layers (Pd-TiC) on the surface of a Pd-foil (thickness 0.1 mm).

2.2. Dependence on the Number of Coating Layers.

The dependence on the number of the coating layers would be quite different if different models are assumed for permeation process as well. In Figure 3 the peak value of the deuterium flux permeating through the Pd foil is a function of the number of the coating layers. It shows a peak-wise feature as well. It was unexpected. When the number of the coating layers increases, the deuterons are supposed to permeate a thicker foil. If its behavior is pure diffusive; then, the deuteron flux is supposed to be a monotonic function. It should decrease when the number of layers increases. However, in Fig.3, the deuterium flux peaked when the number of the layers was equal to 3. Moreover, the flux for 3-layer-foil is still higher than that of 0-layer-foil (i.e. no coating). This behavior can not be explained based on the simple diffusion model.

Figure 3. The peak flux value as a function of the number of the alternative coating layers on the surface of the Pd foil (thickness 0.1 mm)
3. Periodicity of Palladium Lattice

When periodicity is combined with the wave feature of the deuterons we might expect a lot of new coherent phenomena other than the diffusion. However, the de’ Broglie wave length of the deuterons is very small in comparison with that of electrons; hence, one might wonder if the vibration of the lattice might destroy the COHERENCE.

3.1. Debye-Wallet Effect

The theory of electron diffraction might be helpful to solve this problem. Early in 1930’s, when the electron diffraction by crystal lattice was first proposed, the suspects worried about that the random vibration of the crystal lattice might blur the diffraction peaks. It was found later that this blurring effect was a second order effect because the diffraction peaks observed are the average result which would make the first order effect vanished. This second order effect is proportional to the square of the ratio of amplitude of thermal oscillation to the lattice constant. This is called as Debye-Wallet Effect, and has been verified in experiments [12]. The low energy electron diffraction experiments showed that for 100 eV electron beam the diffraction peaks were clearly shown even if the temperature of the crystal lattice approached 400°C [13]. For the deuteron, due to heavier mass we might expect the diffraction and coherent effects for 30 meV deuterons as well, even if the palladium is heated to 140°C.

3.2. Symmetry of Lattice in Different Directions

We must notice that the symmetry of interaction between wave and lattice is different for different directions. Periodicity is from the symmetry of the lattice. For a face-center cubic lattice, it seems symmetrical in three directions, but if we consider the gradient of the deuteron density for the gas-loading cases, the perpendicular direction to the surface of the palladium might be different from the directions parallel to the surface of palladium. When we apply the Bloch Theorem for the wave function of the deuterons, we require the periodicity in the surface layer first instead of the symmetry in 3-directions. The palladium crystal is considered as a combination of many layers: one layer after another layer in the direction perpendicular to the surface. As a result, we have the relation for two components of the momentum in two directions:

\[ k^2 = k_{\|}^2 + k_\perp^2, \]

Here, \( k \) is the total momentum, \( k_{\|} \) is the component of the momentum of the deuteron moving in the direction lying on the surface of the palladium; \( k_\perp \) is the component of the momentum of the deuteron in the direction perpendicular to the surface of palladium. As abovementioned, the periodicity in the surface layer requires that:
\[ k_y = k_0 + \frac{2\pi}{a} n. \]  \hspace{1cm} (2)

Here, \( n \) is an integer; \( a \) is the lattice constant; \( k_0 \) is the eigenvector in the first Brillouin region.

For the permeation in the \( k \perp \) direction, in stead of diffusion coefficient the wave theory would give the reflection, transmission, and absorption coefficients, respectively.

4. Some Qualitative Comparison between Theory and Experiment

Before a quantitative comparison available, we may study some of the qualitative feature for any coherence.

4.1. Temperature Effect

Temperature may change the kinetic energy of the deuteron; hence, the wave length of deuteron. Thus the wave property should be affected by the temperature. In equation (1), the total momentum \( \mathbf{k} \) is determined by the kinetic energy of the deuteron; hence, \( \mathbf{k} \) is a function of temperature. It is known that there are several temperature intervals where we have seen the anomalous phenomena in the D/Pd systems. The famous “Heat after Death” phenomenon appears near 100°C [14]; the nuclear transmutation experiments were done preferably near 70°C [15]; Arata and Zhang’s new Double-Structure experiments were done near 140°C [16], and we discovered the correlation between anomalous deuterium flux and heat flow just near 140-150°C as well [8, 9]. These specific temperatures might be the result of some coherence effects between deuteron wave and the periodicity of the lattice. When temperature increases, both the lattice constant and the kinetic energy of the deuteron may increase. However, the effect of kinetic energy dominates. When more specific temperatures are available we may find their relation with some integers just like that of low energy electron diffraction [12].

4.2. Surface Effect

The wave property should be apparent near the surface layer. The reflection of the deuteron wave on the first surface layer may interfere with the wave reflected from the layer next to the surface layer. The destructive interference might greatly reduce the total reflection wave, and enhance the permeation of the deuteron through the palladium foil. A high gradient of deuteron density would appear near the surface to accommodate this enhanced permeation. This high gradient of deuteron density might be a good region to sustain some coherence. Iwamura’s nuclear transmutation experiment supported this surface effect [15].
4.3. Positive Correlation between Deuterium Flux and Heat Flow

The positive correlation or negative correlation between absorption and transmission implies different physics on the surface of palladium. If we assume that the absorption in palladium leads to the excess heat,( i.e. the heat flow); and the transmission leads to the deuterium flux through the palladium film, then, Fig.1 shows that both the absorption and the transmission may increase together with the temperature. The positive correlation between deuterium flux and heat flow means that the total intake on the surface of the palladium may increase or decrease with the temperature. In other words, the reflection from the surface may change with temperature when the incident number of the deuterium molecules was about fixed by the deuterium pressure. This may be explained as a result of variation of the wave length when the kinetic energy of the deuteron is changing. As a consequence, the coherence between deuteron wave and the palladium lattice is changing with temperature.

In contrary, if a negative correlation between absorption and transmission was observed; then, it might imply the total intake on the surface of palladium may be fixed by the deuterium gas pressure. The absorption might vary with the temperature. Any reduction in absorption would result in the increment of the transmission. Hence, the negative correlation might imply that the reflection from palladium surface does not change with temperature. This is a simple diffusion flux through a Pd film as granular particles. In a word, this positive correlation between deuterium flux and heat flow is an additional evidence to show the wave property of the deuterons near the surface of palladium lattice.

5. Numerical Calculation

5.1. New Paradigm of theoretical description

Reflection, absorption and transmission coefficients are introduced instead of cross-section or life-time here, because we are supposed to set up a model to describe the interaction between the deuteron wave and the periodical lattice well in a steady state. Cross-section is not suitable here, because we are no longer dealing with a beam-target configuration. In the lattice-well-confinement configuration, the reflected wave from the Coulomb barrier may be reflected again by the lattice well. The bouncing back and forth motion happens not only inside the nuclear well, but also inside the lattice well. It is a new kind of resonant interaction between nuclear scale and lattice scale. Hence it is a new paradigm of theoretical description.

We would not use the concept of decay-time of a resonant state here either, because we prefer to study a steady state, i.e. a self-sustaining state maintained by a constant flux. There are three kinds of coherence: the resonance inside the nuclear well; the coherence in multiple scattering of deuteron wave by the symmetric lattice centers; and the coherence between different layers in parallel to the surface layer. In order to simplify the calculation, we start from the simplest configuration, and attempt to answer the most important question: i.e. is it feasible to confine the deuterons inside the lattice well in
order to enhance the d+d fusion reaction rate dramatically at low energy in terms of multiple scattering mechanism.

5.2 Multiple Layer Model

In this simplest model, only one of the three abovementioned coherences is involved. Only the multiple scattering between different layers is considered. The other two coherences inside each layers has been discussed elsewhere preliminarily [17].

A palladium lattice is assumed to be composed by a series of parallel layers in Fig.5. Each layer has 3 parameters to describe its intrinsic nature: i.e. the reflection coefficient, \( R(1) \), the absorption coefficient, \( A(1) \), and the variation of the phase angle, \( \phi \), which gives the phase shift of the wave function after the scattering by this single layer. We have to answer the question: “are we still able to reach a significant absorption coefficient using the coherence of multiple scattering?”, even if the absorption coefficient \( A(1) \) is very small.

We have derived a formalism to describe the multiple scattering effect of \( N \) layers.[18] The reflection coefficient, \( R(N) \), the absorption coefficient, \( A(N) \), for \( N \)-layers may be expressed by \( R(1) \), \( A(1) \), \( \phi \) and \( N \) as follows:

Using quantum mechanics, for a single layer we may write the matrix, \( M(1) \), which connects the outgoing wave function, \( \Psi_{\text{out}}(1) \), and the incoming wave function, \( \Psi_{\text{in}}(1) \) as:

\[
\Psi_{\text{in}}(1) = M(1) \Psi_{\text{out}}(1)
\]  

This matrix is written in the plane-wave representation. For example in the case of outgoing wave only (see right-hand-side of Fig.5),

\[
\Psi_{\text{out}}(1) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}
\]  

then, the incoming wave should be
In general, the scattering matrix for a single layer may be written as:

\[
M(1) = \begin{bmatrix}
\frac{1}{T(1)} e^{-i \phi} & -i \sqrt{T(1)} \\
\frac{i}{T(1)} R(1) & \sqrt{T(1)} e^{i \phi} (R(1) + T(1))
\end{bmatrix}
\]  

Here \( T(1) = 1 - R(1) - A(1) \) is defined as the transmission coefficient for a single layer based on the conservation of the current of probability. The phase angle, \( \phi \), represents the phase change during the scattering in a single layer and during the transition from one single layer to the next layer. The definition of \( M(1) \) in Equation (6) guarantees the symmetry of single layer; i.e. the coefficients of reflection and the transmission are same for the left or right incident wave. When \( M(1) \) is diagonalised as

\[
\begin{bmatrix}
e^{i \alpha} & 0 \\
0 & e^{-i \alpha}
\end{bmatrix}
\]

we have

\[
\alpha = \arccos \left( \frac{M(1)_{11} + M(1)_{22}}{2} \right)
= \arccos \left\{ \sqrt{\frac{1}{T(1)}} \left[ (1 - \frac{A(1)}{2}) \cos(2 \phi) - i \frac{A(1)}{2} \sin(2 \phi) \right] \right\}
\]  

This \( \alpha \) is different from \( \phi \), because \( \alpha \) is calculated for an incident wave which is a combination of two plane-waves traveling in both directions. For the case of \( N \) layers, the scattering matrix equation should be written as

\[
\Psi_{in}(N) = M(N) \Psi_{out}(N)
\]

If we keep the outgoing wave function same as before; then,

\[
\Psi_{out}(N) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}
\]

We may assume
\[ M(N) = \begin{bmatrix} M(N)_{11} & M(N)_{12} \\ M(N)_{21} & M(N)_{22} \end{bmatrix} \]  \hspace{1cm} (11)

Hence,

\[ \Psi_{\alpha\alpha}(N) = \begin{bmatrix} M(N)_{11} \\ M(N)_{21} \end{bmatrix} \]  \hspace{1cm} (12)

Based on matrix algebra, it can be proved that

\[ M(N)_{11} = \frac{\sin[N\alpha]}{\sin[\alpha]} M(1)_{11} - \frac{\sin[(N-1)\alpha]}{\sin[\alpha]} \]  \hspace{1cm} (13)

\[ M(N)_{21} = \frac{\sin[N\alpha]}{\sin[\alpha]} M(1)_{21} \]  \hspace{1cm} (14)

The reflection coefficient, penetration coefficient, and the absorption coefficient may be written as the function of the elements of the scattering matrix:

\[ R(1) \equiv \left| \frac{M(1)_{21}}{M(1)_{11}} \right|^2 \]  \hspace{1cm} (15)

\[ T(1) \equiv \frac{1}{\left| M(1)_{11} \right|^2} \]  \hspace{1cm} (16)

\[ A(1) \equiv 1 - R(1) - T(1) \]  \hspace{1cm} (17)

The similar definition is valid for \( N \) layers

\[ R(N) \equiv \left| \frac{M(N)_{21}}{M(N)_{11}} \right|^2 \]  \hspace{1cm} (18)

\[ T(N) \equiv \frac{1}{\left| M(N)_{11} \right|^2} \]  \hspace{1cm} (19)

\[ A(N) \equiv 1 - R(N) - T(N) \]  \hspace{1cm} (20)

An important conclusion may be drawn from this very general relationship between \( M(N)_{21} \) and \( M(1)_{21} \) (equation (14)): when the reflection rate for single cell is not zero; the total reflection rate for \( N \) cell might be zero as long as
\[
\frac{\sin[N\alpha]}{\sin[\alpha]} = 0 \tag{21}
\]

In physics, this is the result of destructive interference among all the reflected waves. At the same time \(R(N)=0\) implies \(T(N)\to 1\) when there is no absorption. It means a constructive interference among all the propagating waves inside \(N\) layers which enhances the penetration rate greatly. The conservation of the probability guarantees the eventual penetration after all the reflections and penetrations in layers.

Now we may introduce a small absorption coefficient, \(A(1)\ll 1\), for a single layer. Every time the deuteron flux passing through a single layer would be absorbed by a fraction of \(A(1)\). The multiple scattering causes a lot of scattering among all these layers before the deuteron flux finally leaves palladium. The total absorption, \(A(N)\), would become a greater number if the deuteron flux is bouncing back and forth many times inside the multiple layers. Figure 6 is a numerical result for the case of \(A(1)=0.01\), \(N=20\). \(R(1)\) is assumed to be equal to \(T(1)\) for simplicity. The abscissa is the phase angle variation for each layer, \(\phi\). It depends on the distance between two adjacent layers also. The ordinate is the three coefficients, \(A(N)\), \(T(N)\) and \(R(N)\).

![Figure 6. The total absorption coefficient, \(A(N)\), transmission coefficient, \(T(N)\), and reflection coefficient, \(R(N)\) for the case of 20-layers with \(A(1)=0.01\) for a single layer](image-url)

6. **Discussion**
6.1. Positive Correlation between total absorption and transmission.
The solid line, $A(N)$, and the dash-dot line, $T(N)$ reach the peak and valley at the same position. This is just what we expected for a deuteron wave which is reflected from the surface of the palladium layers. When the reflected wave is minimized (the dotted line, $R(N)$) reaches the valley), the wave entering multiple layers is maximized. Hence, both the total absorption, $A(N)$ and the total transmission, $T(N)$ reach the peak.

6.2. The maximum value of $A(N)$
The maximum value of $A(N)$ is more than 0.5 although the absorption for a single layer, $A(1)$, is only 0.01. Since $N=20$, this implies that in average the deuteron would pass through each single layer more than 2.5 times. This is what we expected also. The multiple layers play a role of confinement of deuterons which experience the bouncing back and forth motion inside the palladium before the deuteron flux finally penetrates the multiple layers.

6.3. The minimum value of $A(N)$
The minimum value of $A(N)$ is a little bit less than 0.2. It implies that some of deuterons are reflected out before they reach the 20-th layer.

6.4. boundary for the phase angle
There is a clear boundary for the phase angle, $\phi$. For $(\pi/8) < \phi < (3\pi/8)$, the three total coefficients are oscillating, but beyond this interval, they are decaying or growing monotonically. This behavior is expected from the coherence as well. The phase angle, $\alpha$ in Eq.(8), includes both the information for single layer($A(1)$) and the information for multiple layer($\phi$). When $A(1) \rightarrow 0$, $\cos \alpha$ in Eq.(7) is mainly a real number. However, $\alpha$ may become a complex number when $|\cos \alpha| > 1$. It is noticed that even if $A(1) \rightarrow 0$, $\phi < (\pi/8)$ or $(3\pi/8) < \phi$ just makes $|\cos \alpha| > 1$. This makes $\alpha$ an imaginary number, which results the monotonic behavior of $A(N), T(N)$ and $R(N)$. For $(\pi/8) < \phi < (3\pi/8)$, $|\cos \alpha| < 1$; hence, $\alpha$ is mainly a real number with a small imaginary part ($A(1)\ll 1$). Thus we expect that these three coefficients $A(N), T(N)$ and $R(N)$ would oscillate according to Eq.(7).

7. Concluding Remarks

The coherence between the deuteron wave and the periodic structure of the multiple layers may explain the positive correlation between the excess heat and the deuterium flux near the surface of the palladium. We may use this coherence to confine the deuteron wave inside the multiple layers in order to enhance the fusion reaction rate in the metal deuterides.
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