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Collision Between Two Deuterons in Condensed Matter: IonTrap Mechanism

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Abstract

In this paper is studied the behaviour of ions confined by means of quadrupolar electro-dynamic containment around palladium lattice tetrahedral sites. Ion confinement in a quadrupolar trap is known to be strongly influenced by the initial conditions and trap parameters. The considered system is a lattice ion trap for deuterons, supposing that over a certain concentration they occupy the tetrahedral sites. The electron motions seem to have a dominant role in the dynamics of two deuterons moving around such lattice sites. A mathematical model allows us to describe, with a computer simulation, the deuteron dynamics and reveals an approach mechanism that could strongly decrease the mean distance between two positive charges embedded in a lattice.

1. Model description

Over the past forty years, several authors have investigated electro-dynamic containment of charged particles in a quadrupole trap [1-3]. Our intention in this paper is to develop a preliminary classical study of the dynamics of two deuterons moving within the Pd lattice space around tetrahedral sites, by considering a remarkable similarity between the above mentioned quadrupole radio-frequency traps and the palladium lattice structure. Several features of the palladium-hydrogen system indicate that the hydrogen isotopes (e.g. deuterium) exceeding the atomic ratio x=D/Pd=0.8 have a distinctive kind of interaction with the host lattice. Experimental data [4] indicate that above threshold (x=0.8) the D diffusion coefficient increses steeply by almost two order of magnitude. A suddenly increase of the diffusion coefficient is expected if the energy barrier between two allowed positions decreases. The decrease of the energy barrier could be due to deuterons moving, for x>0.8, from the octahedral sites to the tetrahedral ones. In the following we will assume that over the threshold x=0.8 at least a fraction of deuterons moves from octahedral sites to tetrahedral ones [5,6]. In the proposed model the authors suppose that the alternating signal of a lattice radio-frequency trap can be generated by the motion of electrons close to te Fermi energy. The electron motion can be traced back to an oscillating electronic cloud that produces an electric field. Fig. 1 shows the palladium lattice cell. The octhaedral sites are in the middle between the vertex of the cubic structure. The tetrahedral sites, that could be available for deuterons above x=0.8 [5,6] belong to the intersection between the (101) and the $(10\bar{1})$ planes. We can imagine a similarity between a quadrupolar ion trap and the system shown in Fig.1. It can be shown [5] that the e.m.

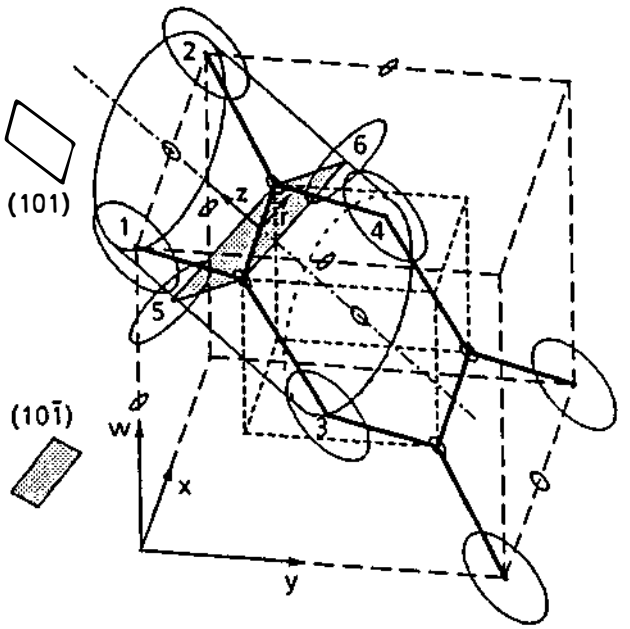

Fig.1 Palladium-Deuterium lattice cell.101 plane and its orthogonal plane (10$\bar{1}$) (dashed area). A similarity can be envisaged between the quadrupolar ion trap and the system shown in the figure. Cylindrical symmetry of the "lattice ion trap"

coupling of oscillators minimize the energy, i.e. the collective motion of N identical oscillators is amplified if compared with to their incoherent interaction. We start considering electronic clouds oscillations having the same phase and the same orientation in both planes (in their coherence domain). For simplicity's sake we consider that the charges acting in the (101) plane are the midway between Pd atoms 1 & 2, and 3 & 4 (see Fig.1) and the charges acting in the (10$\bar{1}$) plane are just the atoms 5 and 6. A simplified two–dimensional representation of the system can be carried out considering the projection in the w-y plane of the spatial electronic cloud oscillations around the Pd atoms. We see that their displacements in both (101) and (10$\bar{1}$)planes are oscillations of the charge density (see Fig.2a, 2b) producing an alternating potential difference that generates an electric field. Then E^{101} and $E^{10\bar{1}}$ in the [101] and [10$\bar{1}$] directions respectively, are the effective components of the electric field for ions dynamics. If we suppose that the electron clouds move at random, then as the oscillation direction moves away from the plane direction (see Fig. 2b) the oscillating charge density decreases within the plane and therefore also the signal across the plane is reduced. This effect can be described by introducing a random factor (ranging between zero and one) in the peak signal. The electric field in each plane acheives its maximum value when it is minimum in the other one and vice-versa because of the orthogonality between the planes: the maximum value of the peak signal for one plane is obtained when the oscillation takes place along the plane direction itself, as can be seen in Fig 2a. Such a situation leads to sinusoidally time varing forces whose strengths are proportional to the distance from a central origin. The trap can be considered to have cylindrical symmetry as shown in Fig.1. The expression for the alternating signal can be derived from the circular symmetric potential distribution [1]. For the system under consideration the field intensities can be obtained by differentiating the potential distribution (and introducing both the coefficients taking into account the effective value of the peak signal in both planes due to the oscillation direction and the possible

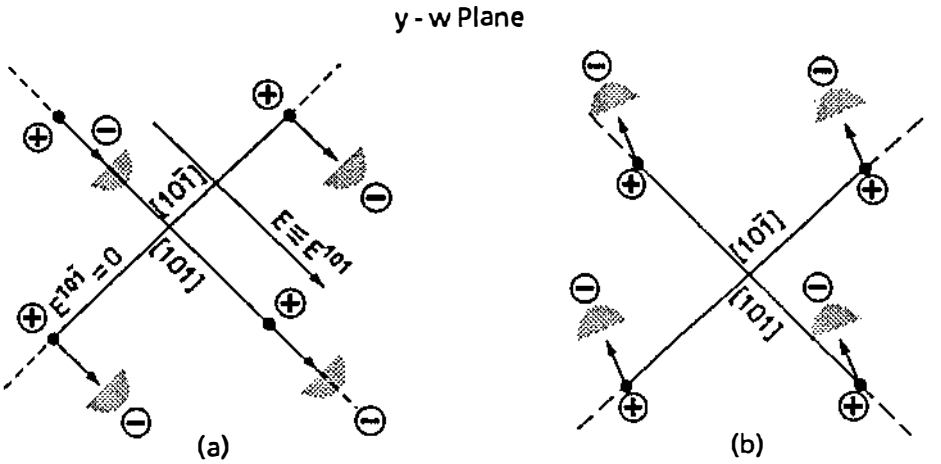

Fig. 2 (a,b) Two-dimensional representation of the alternating signal

shift).Let $E_z = E^{101}$ and $E_r = E^{10\bar{1}}$ then:

$$E_r = -(1-\alpha)V_{acr}\cos(\Omega t + \frac{3}{2}\pi)\frac{r}{r_0{}^2}$$
$$E_z = 2\alpha V_{acz}\cos(\Omega t + \phi)\frac{z}{r_0{}^2} \qquad (1)$$

where V_{acr} and V_{acz} are the r and z ([10$\bar{1}$] and [101] directions respec-tively) peak values of the alternating signal having angular frequency Ω, r_0 is the trap characteristic length (the radius or the length from the simmetry point that are equal in this case), r and z are the relative coordinates of two deuterons moving in the trap, α is a random number, ranging between 0 and 1 taking into account the direction of oscillation, and φ is a random phase shift that is equal to zero if we imagine collective organized oscillations of the electronic clouds (α and φ can also change after a time interval of the order of the oscillation period).Considering both the coordinates, and introducing the following dimensionless variables $\bar{r} = \frac{r}{r_0}; \bar{z} = \frac{z}{r_0}; x = \frac{\Omega t}{2}$, the balance of the forces leads to:

$$\frac{d^2\bar{r}}{dx^2} = -\frac{2}{m\Omega^2 r_0{}^2}\frac{dE_b}{d\bar{r}} + \frac{4}{m\Omega^2}\bar{r}[e^2\frac{1}{(r^2+z^2)^{3/2}} + \frac{(1-\alpha)eV_{acr}}{r_0^2}\cos(2x+\frac{3}{2}\pi)]$$
$$\frac{d^2\bar{z}}{dx^2} = -\frac{2}{m\Omega^2 r_0{}^2}\frac{dE_b}{d\bar{z}} + \frac{4}{m\Omega^2}\bar{z}[e^2\frac{1}{(r^2+z^2)^{3/2}} - \frac{2\alpha eV_{acz}}{r_0^2}\cos(2x+\phi)] \qquad (2)$$

where e is the electron charge. The terms on the right side of Eq. (2) are due to the damping force, the Coulomb interaction and to the trap force respectively. The damping force could be evaluated as the gradient of the energy barrier whose shape is unfortunately unknown. Therefore in this preliminary description the damping term in the Eqs.(2) is simply evaluated as average gradient of the energy gap $\Delta E_b / r_0$ (being ΔE_b

the energy barrier,~0.2 eV). The initial conditions have to be included to describe the relative position of the two deuterons, travelling towards the trap, and their initial velocity. The frequency of the alternating signal can be evaluated by means of the approximation to an ideal electron plasma [5]. In this calculation we shall assume, as mentioned above, that only the electrons close to the Fermi level (4d-5sp bands) partecipate to the oscillations ($n = 6.8\times10^{23}$). The peak value of the alternating signal can be calculated on the basis of the electric field, in the classical approximation, associated with the plasma oscillation: $V_{acr,z} = 4\pi n e \eta^2$; where η is the maximum distance between the positive and negative centres of charge during the oscillations: i.e. the distance between the Pd atoms (here η =2.83 Å and $V_{acr,z} \sim 10^3$ V).

2. Results and Conclusions

The computer simulation allows us to investigate the system's sensitivity to the initial conditions and to obtain a preliminary correlation between the lattice state and the *collision* between two deuterons. The lattice cell parameters used in the simulation have been obtained from the lattice constant for the β phase. The **Fig. 3** shows the evolution of the distance between two deuterons versus the dimensionless time α=constant and φ=0. Fig 3a shows the situation when it is considered a Coulomb interaction, whereas Fig. 3c shows the analogous by considering a Thomas-Fermi screened potential. The closest approach, within the investigated time interval is ~0.1 Å but after one *collision* one of the particles escapes from the trap. Fig. 3b shows the distance evolution (assuming a Coulomb potential) with a different choice of the initial conditions. In this case no *collision* occurs. Figure 4a shows the evolution of distance between the two deuterons vs the dimensionless time by assuming the same conditions as the case described by Fig. 3b, whereas the Fig. 4c shows the situation by considering an electron plasma density reduced of 10%. We can see (in the enlargement of the *collision* region) that because of the reduction of the plasma frequency and of the peak value of the signal (see Eqs (6) and (8)) the minimum distance of approach increases. This effect is not negligible in terms of nuclear interaction probability. Thus this analysis reveals that an increase of the Deuterium/Palladium loading ratio, with an associated increase of the electron plasma density plays an important role in the *collision* event. Fig 4b show the situation with the same initial condition of the case described by Fig. 3b but assuming a T.F interaction potential. From the numerical calculations it results that, under the same conditions, the minimum distance between deuterons increases if the electron clouds oscillate with a time dependent orientation (even if it is always of the order of 0.1 Å). The components of the electric field (1) are still valid in this case because the time domain has been divided in sub-intervals where α is constant. In this case the integration is carried out taking as initial condition for each sub-interval the final condition of the previous one. Even if the calculated distances between the deuterons can only be considered indicative, the model gives the interesting result that, the deuterons, because of the electronic oscillations within the Pd lattice, can approach each other up to distances of the order of a fraction of one angstrom; therefore overlapping deuteron wave functions can be obtained at low energy in condensed matter under a variety of scenarios and hypotheses concerning the trap mechanism. Also, the calculations show that the two nucleus remain close together for a time long compared with the nuclear reaction time (~10^{-15} s against ~10^{-21} s). In addition to the cases discussed here, several other boundary conditions have been used giving similar behaviour of the deuterons. The combined effects of the trap force, the trostatic interaction, non linearity, and the damping produce, under proper conditions, an interesting effect of *collisions* between the particles. Besides it is possible that a nuclear

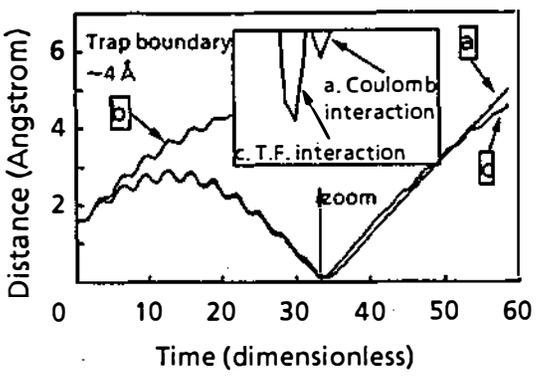

Fig. 3 evolution of the distance between two deuterons (α=constant, φ=0). Fig 3a (Coulomb interaction), Fig. 3c (Thomas-Fermi screened potential). In both cases the initial dimensionless coordinates are r(t=0)=0.001, z(t=0)=1.1, and the initial dimensionless relative velocity components are r'(t=0)= =0.001 and z'(t=0) =0.12. Fig. 3b shows the distance evolution (assuming a Coulomb potential) with a different choice of the initial conditions: r(t=0)=0.001, z(t=0)= 1.1, r'(t=0)=0.125, z'(t=0) = 0.12.

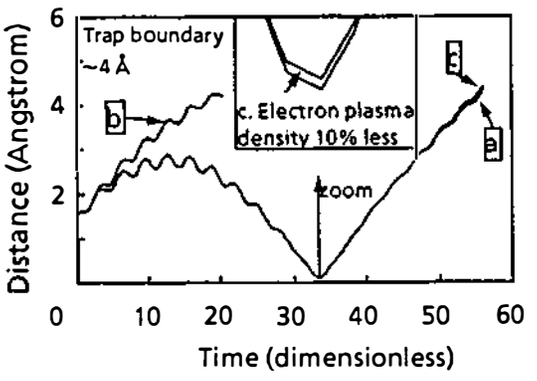

Fig. 4a evolution of distance between the two deuterons (conditions of Fig. 3c), whereas the Fig. 4c shows the situation with an electron plasma density reduced of 10%. Fig. 4b show the situation with the same initial condition Fig. 3b but assuming a T.F interaction potential.

reaction could proceed in matter differently from in vacuum, if coupling with a radiation field in the nuclear transition probability is taken into account. Furthermore we observe that the condition for close approach between two particles is produced by proper values of the plasma electrons density, cell trap geometry and lattice state; therefore it is not impossible that a similar dynamics can be obtained by using host materials different from palladium. The model highlighs that a face centred lattice plays a fundamental role in deuteron confinement and dynamics. It should be observed that the proposed mechanism is not necessarily a bulk mechanism but can take place also in a material region very close to the surface, within several hundred angstroms. Quantization should be carried out among the future developments.

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