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BINUCLEAR ATOMS AS FUSION PRECURSORS IN A HOT CLOUD

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ABSTRACT

Deuteron-deuteron fusions were claimed by a Brookhaven group to result from the impact on deuterated surfaces of clusters of 25 - 1350 D_2O molecules with energy up to 300 keV. The collective motion in the impact region is tentatively assumed to be responsible for these fusion events. The number of involved atoms is of the order of 10^4, with a mean energy of some electronvolts. The model is able to reproduce qualitatively the Brookhaven data according to an Arrhenius plot, with an activation energy $E^* \simeq 2\,E_0$, where E_0 is the hydrogen ionization energy. At this energy an activated precursor is postulated to be synthesized; it can tentatively be identified as the binuclear atom $(D^+ - D^+)2e^-$.

1. INTRODUCTION

A Brookhaven collaboration has recently presented surprising results concerning the detection of D - D fusion products in TiD targets following bombardment with $(D_2O)_n$ clusters $(25 < n < 1350)$ [1]. The evidence of fusion events was successively extended using perdeuteriopolyethylene $\{ CD_2 - CD_2 \}_n$ and $ZrD_{1.65}$ targets [2].

The experimental arrangement utilized in the first work [1], though apparently simple, was subjected to criticisms, since in-flight fragmentation or evaporation after mass separation or poor mass separation of the clusters may reproduce the observed fusion rate and its energy dependence [3]. Indeed, a single D^+ ion per cluster, accelerated at a few kiloelectronvolts, can reproduce the Brookhaven results without advocating any new phenomenon.

In order to identify a possible fragmentation of the cluster in light fragments, the use of a pulsed beam and the detection, by a coincidence technique, of the time of emission of the reaction products was proposed. The fragmentation of the cluster into light ionized fragments is indeed characterized by the arrival on the target of these fast fragments some microseconds before the cluster arrival [4]. A coincidence set-up in the microsecond range should detect these early events, if any, and attribute them to a trivial fragmentation process and not to a new, at the moment unexplained, phenomenon.

A cluster-impact experiment in the pulse mode with a repetition frequency in the hertz range was executed by another group [5]. No protons were revealed following the impact of 100 – 150 keV pure deuterium clusters, constituted by 200 - 300 D atoms, on $TiD_{1.7}$ and $\{ CD_2 - CD_2 \}_n$ targets. Though this part of the experiment does not confirm the Brookhaven results, the Brookhaven collaboration has very recently obtained positive results in the pulsed mode too [6].

Another possible source of experimental error in the Brookhaven set-up is due to deuterium atoms backstreaming from the target under cluster bombardment. Backstreamed atoms

could successively be ionized and accelerated in the column onto the target [7].

However, already in the reply to this criticism [8] and mostly in the second work [2], the Brookhaven group produced a lot of evidence which seems to exclude fragmentation or evaporation, poor mass separation, or backstreaming. In the following we assume the unrestricted validity of the Brookhaven results.

We note that artifacts, if any, are due to the presence in the beam of fast atoms and that in the fusion events originated by, say, 10 keV D^+ impinging onto the target, the energy of the protons emitted toward a detector placed at a scattering angle around 125° is about 70 keV less than the energy, 3.02 MeV, of protons emitted in fusions promoted by low energy deuterons. *This shift in the proton energy spectrum should easily be detected if the detector is properly placed and if its resolution in the experimental set-up is sufficient* — these considerations should be able to rule out, or to confirm the presence of, all hypothesized artifacts.

2. DISCUSSION OF BROOKHAVEN RESULTS

The Brookhaven results are particularly surprising if plotted as a function of the kinetic energy E_D of a deuterium atom in the cluster, $E_D = (M_D/nM_{D_2O})E \simeq 0.1E/n$, where E is the cluster energy and M_X is the mass of the molecule X. Indeed, the comparison of the data collected at constant E and variable n with the data taken at given n and variable E shows that the fusion yield per deuteron y is not a single-valued function of E_D, but depends also on cluster composition [9]; this fact is completely inconsistent with the view of fusions produced by independent collisions of $2n$ impinging deuterons.

In order to remove this contradiction, we are led to consider in greater detail the impact of the cluster on the target using a model which describes the collective motion of the atoms in terms of hot cloud formation. If the number of atoms in a cluster is high enough, the collisional cascades produced by single atoms superimpose and form a unique cascade so dense to be treated as a hot cloud; the duration Δt of this phenomenon and the number N of involved target atoms is much larger than the values estimated by Beuhler et al. [1], i.e. $\Delta t \approx 10^{-11}$ s vs 10^{-13} s, and $N \approx 10^4$ vs 10^3 [10,11]. A much larger number of deuterons can therefore interact for a much longer time Δt, however with a lower mean kinetic energy E_{kin} than assumed by Beuhler et al. If a phenomenon able to activate fusion at low energy exits indeed, it is plausible that the relevant parameter for the description of the phenomenon is no longer E_D, but the cloud temperature T, assumed to be related to E_{kin} by the usual formula $E_{kin} = \frac{3}{2}k_B T$, where k_B is the Boltzmann constant [12].

If we assume for the moment that only deuterium atoms are able to inject useful energy into the cloud, the average kinetic energy in the cascade is given by

$$E_{kin} = \eta(4/20)E/(2n + N), \tag{1}$$

where η is the fraction of the impinging energy which is not lost in electronic collision. Simulations carried out with the MARLOWE code give η in the range 0.6 – 0.8 (tentatively we assume $\eta = 0.7$) and suggest that most of the useful energy in the cascade is indeed injected by the deuterium atoms, owing to their identical mass with the target atoms [13]. By contrast, the oxygen imparts most of its energy to titanium, so that this energy deposition seems to be decoupled from the deuterium cloud energy. In a way, the particular choice of projectile and target of the Brookhaven group, though scarcely efficient in terms of deposition of useful energy, gives rise to a very simple situation to be modeled, in which only deuterium atoms or ions are involved. The small fraction ($\simeq 4/20$) of incoming energy useful to promote fusion events delineates a framework very different from the one presented by Echenique et

al. [14] in which the deposition to deuterium atoms in the target of the whole cluster energy is assumed, so that some high energy deuterons in the upper tail of the resulting energy distribution could promote fusion events according to conventional nuclear physics.

From eq. (1) E_{kin} can be considered independent of n only for $2n \ll N$. Since the data of Beuhler et al. are nearly constant from $n = 10^2$ to $n = 5 \times 10^2$, a first underestimate of N, $N \gg 10^3$, results. In order to take into account the data at variable E for fixed n, we note that an assigned value of N in eq. (1) combined with the variation with E which results from the experimental data allows the corresponding theoretical fusion yield $y(n, N; E)$ to be calculated. The value $N = 10^4$ fits adequately the experimental data and is in accordance with the results of molecular dynamics simulations [10] and with evidence from silicon amorphization [15].

While the two curves are able to describe in a satisfactory manner the data for high n, they cannot be extended in the low n region. In this region E_D is responsible for a projected range R_p of the deuterium atoms larger than the diameter L of the collisional cascade; this suggests that N should vary as

$$N = N_0(1 + R_p/L) = N_0(1 + \beta E/n) \tag{2}$$

where R_p/L has been assumed proportional to E/n through the coefficient β. The description of the cascade can be further refined taking into account the increase of the electronic energy loss at deuterium energy higher than 0.5 keV and the sparse collisional cascades formed by small clusters. These phenomena can in a first approximation be described with a reduced increase of E_{kin} for increasing E and decreasing n. The global effect is similar to the one described by eq. (2),

$$E_{kin} = \eta(4/20)E/[2n + N_0(1 + \alpha E/n)] \tag{3}$$

where α (which includes β) is now a parameter to be estimated by fitting the experimental data.

Using this formula, all the data may be reported in an Arrhenius plot [9]. The best fit of all data gives: $N_0 = (10 \pm 0.5)10^3$, $\alpha = 1.8 \times 10^{-2}$ keV^{-1}, and $E^*/\eta = (33 \pm 2.5)$ eV. Interestingly enough, the estimate $N_0 \simeq 10^4$ is in a satisfactory agreement with those of ref.s [10,11,15], thus underlining an intrinsic coherence in the developed picture.

Though the hot cloud model explains the behaviour of fusion rate vs T and therefore vs n and E, showing that with a good approximation this rate is a function of $E/[2n + N_0(1 + \alpha E/n)]$, however, it cannot explain the extremely high values obtained by the Brookhaven group. Indeed, taking $\eta = 0.6 - 0.8$, E^* results in the interval $20 - 26$ eV, i.e. a value too low to be associated with the overcoming of the internuclear Coulomb barrier. However, the fairly accurate description of all data obtained with the hot cloud model makes us confident in the search of a physical significance of E^*. In this respect it is interesting to note that the value of E^* is approximately twice the ionization energy E_0 of the deuterium atom, so that an atomic, rather than nuclear, phenomenon seems to drive the fusion events. We therefore assume that at the energy E^* a metastable precursor in a favorable situation to fuse is formed.

Further considerations must be taken into account for the development of the model. First of all, in the considered energy range the deuterium atoms move in the target in an atomic rather than in an ionic form, thus allowing, for an assigned kinetic energy, closer nucleus-nucleus encounter and hence higher fusion yield. This consideration is based on the formula of ref. [16] giving the effective charge on hydrogen and deuterium at various kinetic energies; for instance the effective charge is $0.18e$ at 2 keV and $0.13e$ at 1 keV (e is the

unitary charge). Secondly, the interaction potential of two deuterium atoms must take into account the screening effect of the orbiting electrons; we assume that screening is described by the Debye potential

$$U(r) = (e^2/r)\exp(-r/a) \tag{4}$$

where a is a screening length. Historically, potential (4) was used in the description of most of screening problems concerning the penetration of atomic particles through matter [17]; this description is accurate enough at separations of the order of the Bohr radius a_0. For hydrogen $a = a_0$, and for two interacting atoms with atomic numbers Z_1 and Z_2 the Firsov composition rule, $a = a_0/(Z_1^{1/2} + Z_2^{1/2})^{2/3}$, holds true [18]. This rule is routinely used in the calculation of the stopping powers and of the damage effects for practically all projectiles in solids [16].

In the description of the interaction of two deuterium atoms, large and small separations must be independently considered.

Large separation. For large D - D separation, only electrostatic effects are important and the random relative spin orientation is mute in the description of the system. The total energy of two separate repelling atoms is therefore:

$$E_{(D^+)e^-+(D^+)e^-}(r) = (e^2/r)\exp(-r/a) - 2E_0 \quad [E(\infty) = -2E_0] \tag{5}$$

Small separation. At kinetic energy higher than 27 eV the nuclei can approach at distances lower than $0.5a_0$, so that the D - D system can no longer be treated as formed by two moderately perturbed atoms. In a way, the nuclear separation admits a stationary electronic configuration resembling that of the helium atom so that the system can be regarded as a $(D^+D^+)2e^-$ binuclear heliumlike atom. Its total energy can be estimated by the formula

$$E_{(D^+D^+)2e^-}(r) = e^2/r - (E_1 + E_2 - 2E_0)\exp(-0.46r/a_0) - 2E_0 \tag{6}$$

where E_1 and E_2 are the first and the second ionization energies of the helium atom; the term $\exp(-0.46r/a_0)$, which spans from 1 to 0 for r ranging from 0 to ∞, is derived by a least square procedure from the curve which describes the electronic energy of the molecular ion H_2^+, for which an exact theory exists. It must also be noted that eq. (6) matches within 1 eV in the interval $0.4 - 0.7a_0$ the most accurate calculations available [19] for H_2.

In the paraheliumlike case (antiparallel spins), $E_1 = 24.58$ eV and $E_2 = 54.40$ eV; for the orthoheliumlike case $E_1 + E_2 = 59$ eV. These situations corresponds to the two stationary states of the system. Because of the random spin orientation, however, the state of the system is generally a non-stationary linear combination of orthohelium and parahelium states; correspondingly the electronic energy of the system will assume an intermediate, spin-dependent, value.

Calculating the total energy of the system by means of eq. (5) for $r > 0.6a_0$ and of eq. (6) for $r < 0.5a_0$, the energy of the system must have a minimum in the interval $0.4a_0 < r < 0.5a_0$ (the system is unstable with respect to dissociation in all its components for $r < 0.4a_0$) provided that the relative spin orientation is not too far from the antiparallel one, so that a metastable configuration must exists in this separation range. Hence, the D - D collision in a suitable energy range and with an appropriate impact parameter leads to a nuclear configuration for which the total energy has a relative minimum. If a third body is able to absorb a small fraction of the original kinetic energy, then the colliding deuterium atoms can be bound in a binuclear heliumlike atom. This metastable state can decay either by

dissociation or by fusion. The stability of the heliumlike configuration, the *metastable precursor*, is higher the higher the activation energy for its dissociation; to estimate this energy a knowledge of the spin orientation distribution and a detailed calculation around $r = 0.5\,a_0$ is necessary. In any case, in the most favourable conditions the binuclear atom allows much longer interaction times for the two deuterium nuclei than an ordinary collision, so that extraordinarily fusion rates are no more surprising.

A possible consequence of the existence of the metastable precursor concerns the suggestion to utilize coincidence techniques in the microsecond range as a signature of the arrival of the different projectiles. However, if the observed extraordinarily high fusion rates are indeed due the formation of a metastable precursor, the fusions are no more prompt and decay exponentially with time according to the mean life of the precursor. The most recent Brookhaven result with pulsed beam does not totally clarify this point.

General semiquantitative considerations based on the structure of the collisional cascade allow the identification of classes of projectiles and target materials to be used in order to enhance the hot cloud temperature and hence the fusion rate. The best choice is obtained by combining as light as possible targets with very heavy projectile not containing light atoms. Volatile heavy molecules allow the preparation of very simple sources, surely useful when they are maintained at high potential as it happens in ion implanters. These sources prevent from artifacts originating from in-flight fragmentation or evaporation of ionized deuterium fragments from the cluster; as far as the experimental set-up is concerned, an ion implanter with mass selection after ion acceleration also protects the experiment from in-flight fragmentation. An activity in this field is in its preliminary stage.

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