Cluster-Impact Fusion

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We present a model for the cluster-impact-fusion experiments of Buehler, Freidlander, and Friedman. Calculated fusion rates as a function of bombarding energy for constant cluster size agree well with experiment. The dependence of the fusion rate on cluster size at fixed bombarding energy is explained qualitatively. The role of correlated, coherent collisions in enhanced energy loss by clusters is emphasized.

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In an important recent series of experiments, Buehler, Friedlander, and Friedman[1] (BFF) have demonstrated a large yield of fusion events occurring in collisions of D_2O clusters with TiD targets. Clusters of 25–1000 molecules are accelerated to the 300-keV range. The yield of fusion events, as observed through the reaction branch that produces tritium at 1 MeV and a 3-MeV proton, is more than 10^{10} times larger than that expected from the fusion cross section for deuterium atoms with the typical relative velocities of less than 0.1 a.u. that are provided by the cluster. For fixed accelerating energy, the fusion yield as a function of cluster size has a maximum near 200 D_2O molecules. For fixed cluster size the number of fusion protons measured increases strongly with total cluster energy. The authors suggest that these high fusion yields may be due to a greatly enhanced deuteron density produced in the cluster-impact region in the target.

We propose a mechanism based on the large energy and density fluctuations expected in swift-cluster impact. When a D_2O cluster strikes a solid surface the resulting many-body collisions give rise to a small fraction of deuterium atoms accelerated to high translational energies. The D-D fusion cross section increases by over 20 orders of magnitude as the relative speed ranges from 0.1 to 1 a.u. (Ref. 2). Thus a small number of high-speed collisions between deuterium (D) atoms can lead to a large enhancement in the number of fusion events. It is pertinent to note that a 300-keV cluster of fifty molecules has a speed of ~ 0.1 a.u., while if this same energy is given to a single molecule its speed is roughly 1 a.u. and such a particle would have a high probability of causing fusion upon impact. Thus great care was taken in the experiments of BFF to eliminate small-mass clusters from the incident beam. We show here that the small number of D atoms excited to high energies during impact is sufficient to explain the measured fusion rates. The increase of the yield with cluster energy is well predicted by our model, and the dependence on cluster size is explained. We show that the energy dependence of the measured fusion rate does not agree with that found by assuming that the entire energy of a cluster is given to a single D atom.

The fusion rate per D atom may be written

$$\mathcal{R} = \tfrac{1}{2}\eta\langle\sigma v\rangle , \tag{1}$$

where v is the D-D relative speed, η is the density of D atoms, σ is the D-D fusion cross section, and the brackets signify an average over the appropriate speed distribution. A good approximation to the cross section is given by[1]

$$\sigma(E) = (S/E)e^{-A/\sqrt{E}} , \tag{2}$$

with $S = 5.5\times 10^{-23}$ cm^{2}keV and $A = 31.28$ keV$^{1/2}$. We show that a very simple and straightforward model gives an estimate of $\mathcal{R}$ that is consistent with observations. Because of the extremely small cross section of Eq. (2) at low velocities, only those deuterons elevated to high energies in the impact process will participate appreciably in fusion reactions. We assume that the high-energy tail of the velocity distribution function can be well represented by the exponentially decreasing behavior of the Maxwell-Boltzmann function, and Eq. (1) takes the form

$$\mathcal{R} = \eta\frac{S(2/M)^{1/2}}{E_0^{3/2}\Gamma(3/2)}\int_0^\infty dE\, e^{-E/E_0}e^{-A/\sqrt{E}} , \tag{3}$$

where M is the deuteron mass. We assume $\eta = 1.3\times 10^{23}$ deuterons/cm^3, taking the density to be enhanced by a factor of 2 over the normal value and estimate $E_0 = 500$ eV, assuming that a $(D_2O)_{100}$ cluster energy of 300 keV is shared by ~ 1000 particles in the impact region as assumed by BFF. With these parameters Eq. (3) gives $\mathcal{R}\sim 0.08$ s^{-1}, a value that compares favorably with the figure of 0.1 s^{-1} estimated by BFF from their experimental data assuming a confinement time of 10^{-13} s.

The overwhelmingly major contribution to the fusion rate comes from the small number of D atoms in the high-energy tail of the velocity distribution, and consequently the result is very sensitive to the choice of E_0. Taking E_0 as 300 eV rather than 500 eV reduces $\mathcal{R}$ by

more than an order of magnitude and increasing E_0 to 1 keV augments $\mathcal{R}$ by 2 orders of magnitude. Over the range of cluster energies observed in the experiment our model gives E_0 as approximately proportional to the cluster energy. Thus this large increase of $\mathcal{R}$ with E_0 agrees with the observed behavior as a function of incident energy. The dependence of $\mathcal{R}$ on E_0 can be approximated as $\mathcal{R} \sim \exp(-C/E_0^{1/3})$. Numerical calculations from Eq. (3) shown in Fig. 1 give a behavior that compares quantitatively quite well with the published data for a 150-molecule cluster. The results shown as a solid curve were computed for $(D_2O)_{150}$ clusters. They are not changed appreciably if one assumes that the beam contains a distribution of sizes about the assumed value.[3] Figure 1 also shows the fusion rate that would be obtained if the entire cluster energy were given to a single deuteron. This result, the dashed curve, was obtained by normalizing to the measured rate at 300 keV. This energy dependence is definitely not that of the experimental data.

The dependence of $\mathcal{R}$ on cluster size, at constant cluster energy, is also qualitatively explained by this model, again because of the extreme sensitivity to the value of E_0. As the cluster size increases, the same amount of translational energy is distributed over a larger region of the target giving a lower effective energy E_0 of the localized impact spot. According to the arguments of the paragraph above, this lowered E_0 results in a sharp decrease in $\mathcal{R}_0$. On the other hand, if the cluster becomes substantially smaller than 100 molecules, the impact region has dimensions comparable with the mean free path between collisions. This implies that the energy is dispersed, resulting in far fewer high-energy D particles, and consequently a dramatic drop in fusion rate. This description agrees nicely with the observation of maximum fusion rates for 300-keV clusters of 100–600 molecules with a sharp dropoff for clusters larger or smaller. Note that for the smallest clusters used by BFF [$\sim(D_2O)_{25}$], and assuming a uniform average energy per nucleus, the estimated rate of directly generated fusions due to the incidence and slowing down of the deuterons in the target is less than that observed by BFF for a $(D_2O)_{25}$ cluster by several orders of magnitude, and is thus negligible compared with the rates displayed in their Fig. 3.

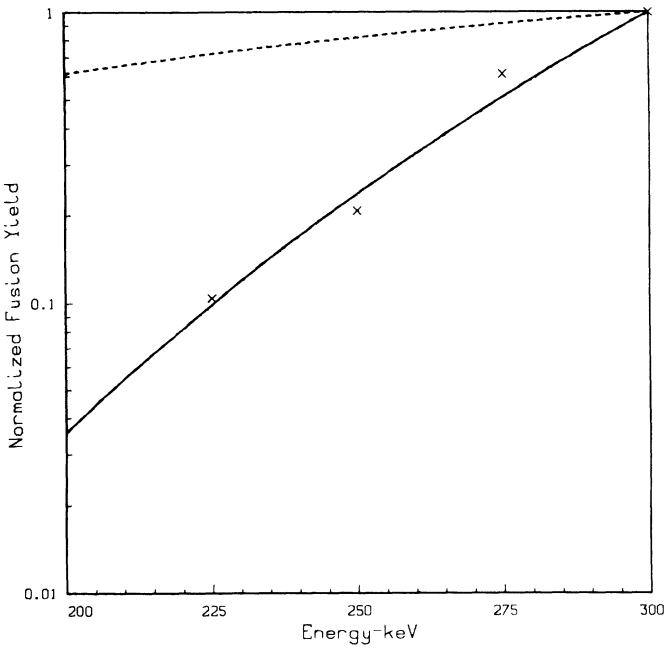

FIG. 1. Fusion rate for $(D_2O)_{150}$ clusters incident on a TiD target vs energy of the cluster. The crosses are the experimental points of BFF (Ref. 1). The data points have been scaled down slightly (Ref. 20). The solid curve was computed from Eq. (3), while the dashed curve was calculated for single deuterons incident on the TiD target, allowing for slowing down in the target.

There has been substantial recent interest in possible enhancement of fusion rates in condensed matter induced by screening of the deuterium Coulomb field by the Fermi electron cloud.[4–7] There appears to be substantial agreement that screening can have a large effect on the cross section for low-velocity D-D interactions, but is insufficient to produce appreciable fusion rates at ambient temperatures.[6,7] Intuitively, one would expect that for the model presented here, screening would play a negligible role since only the high-energy D particles contribute to $\mathcal{R}$ and at such large velocities screening has only a small effect on $\sigma(E)$. Numerical calculations using a screened interaction function[8] show little dependence on screening for values of E_0 above 300 eV.

This model, in spite of its simplicity, appears to do a reasonable job of explaining the experimental results, even to the point of quantitative agreement with fusion rates. However, it should be pointed out that the use of a Maxwell-Boltzmann distribution to estimate the numbers of high-velocity deuterons occurring in the impact process is likely to produce an underestimate of fusion rates. Molecular-dynamics simulations of processes which inject a large amount of energy into small volumes in condensed matter predict that there can be large fluctuations in numbers of high-energy particles as compared with a thermodynamic distribution, particularly during the early stages of interaction.[9,10] Because of the rapid increase of $\sigma(E)$ with velocity, fluctuation enhancements in numbers of high-energy deuterons, even if only over brief periods, are capable of strongly increasing $\mathcal{R}$.

A swift cluster of atoms interacting with a solid may create large deformations, intricate collision patterns, and particles with very high transient energies. Upon impact the cluster and the target are subjected to drastic perturbations, even when $v \sim 0.1$ a.u. as in the experiments under consideration. Target atoms near the sur-

face experience strongly correlated collisions with entering cluster atoms, while electrons of the cluster tend to be promoted to energy levels above the Fermi level of the target electrons. The cluster itself may deform substantially upon impact. As pointed out by Matthew *et al.*,[11] the hydrodynamical theory of such interactions may not be accurate for the impact speeds considered here. As noted in Ref. 11, at high velocities ($v \gg 1$ a.u.) the penetration of clusters might be regarded in zeroth approximation as the penetration of independent atoms, each described by stopping-power theory. This should be useful for a very rough estimation of the scales of relevant processes. However, realistic evaluation of cluster penetration should account for the possibility of correlated atomic collisions as well as vicinage interactions between pairs, triplets, quadruplets, etc., of atoms in the cluster.[12] Experimental evidence has accumulated in recent years showing strong nonlinear enhancement of secondary-ion and atom emission from solids by swift many-atom clusters compared with that due to monatomic clusters.[11,13,14] Thomas, Oladipo, and Fallavier[14] have analyzed their data on the dependence of secondary-ion emission on the number of atoms in a many-atom cluster at constant velocity in terms of a function that depends on the number of pairs of atoms in a cluster.

In their comprehensive review, Buehler and Freidman[15] stress that the basic physics of cluster impact on solids is not well understood. It appears that, in the velocity range of interest here, clusters lose energy to a target at a rate substantially larger than that calculated from standard single-particle atomic collision theory. They suggest that one aspect of cluster collisions contributing to augmented energy loss is that on the average one expects smaller impact parameters to exist in such impacts than in the impact of a single ion because of the greater rigidity of the internal atoms of the interacting system.

The penetration of a swift cluster may be significantly less than that computed for the range of an isolated particle of the cluster moving in the target. For the clusters used by BFF the mechanisms that contribute to range shortening may be classified roughly as (a) multiple scattering of cluster atoms in the target, (b) intracluster scattering as D and O atoms lose energy at different rates, and (c) correlated cluster-target collisions.

We have estimated the range shortening of D atoms in TiD due to effect (a) above using standard collision theory.[16-18] We find that the path length of a 300-eV D atom in a 300-keV $(D_2O)_{100}$ cluster in slowing to half of its original energy is ~ 84 Å but that the projected range R_p in the entrant direction is only ~ 15 Å. Intracluster D-O scattering (b) is estimated roughly to change R_p only slightly to ~ 14 Å. Thus multiple scattering tends to confine the cluster atoms to regions of the target with dimensions comparable with the cluster size.

We suggest that another interesting feature of the intricate many-body cluster-target interaction relevant to enhanced energy loss is the possibility of strongly correlated coherent collisions (c). For example, consider a single atom with mass M_2 located near the target surface and at constant impact parameter relative to a certain string consisting of n atoms in an incoming cluster. For simplicity, neglect the motion of the atom and its binding in the target during the collision. The momentum absorbed by the selected atom as the string passes may be written $\Delta \mathbf{p} = \int_0^T \mathbf{F}(t)dt$, where T is the time required for the string to pass the atom and $\mathbf{F}(t)$ is the force on the atom at time t. Then one might expect that the energy taken up would be given roughly by

$$n^2 \left| \int_{t_i}^{t_{i+1}} \mathbf{F}(t)dt \right|^2 \Big/ 2M_2 ,$$

where t_i is the time at which the ith atom of the string passes by the target atom. This starkly simplified picture neglects, among other things, the influence of other strings but might well represent an underestimate of the effect of correlated cluster-target collisions. To take very rough account of this mechanism we may simply multiply the nuclear stopping power of the target for individual atoms by $\frac{1}{3}(3N/4\pi)^{1/3}$, where $N \gg 1$ is the number of atoms in the cluster. Using this recipe we find that the 300-eV D-atom projected range is even less than the cluster dimension. Clearly this calculation is only indicative of the actual energy-loss enhancement in process (c). However, this model accounts qualitatively for the relative inefficiency of energy transfer from cluster atoms to target electronic motion in the early stages of the cluster-target interaction that is discussed by Buehler and Friedman.[15] Detailed study of large-cluster energy losses in solids offers a substantial challenge to theory, particularly at velocities $v < 1$ a.u., as in the BFF experiments.

In conclusion, we believe that the experiments of BFF on fusion yield from D_2O-cluster bombardment of TiD targets may be explained by a simple argument involving multiple collisions occurring in cluster impact. The fusion rates per deuteron are computed to be of the same order of magnitude as those estimated by BFF from their data. Further, we advance a qualitative argument to explain the measured count rates as a function of cluster size for constant cluster energy. We point out that the experiments of BFF as well as those of Refs. 13 and 14 raise important questions about cluster penetration at bombarding speeds much greater than the speed of sound in the target but appreciably less than 1 a.u. Computer simulations of large-cluster penetration of the kind pioneered by Harrsion[19] would be very desirable in this connection. The authors are undertaking such an approach.

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