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Interaction of fast C_{60} clusters with a Lindhard gas

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The interaction of a C_{60} cluster with a Lindhard gas of electrons at a density near that of the valence electrons of aluminum is calculated. The calculation includes the charge-state evolution of the ion fragments, the disintegration dynamics, and the interference effects of neighboring ions on the energy loss. Enhancement in the energy loss is calculated and it is predicted that this can be observed experimentally for sufficiently thin targets. In addition, the dependence of the energy-loss enhancement was studied as a function of cluster kinetic energy and target density.

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The interaction of energetic beams of clusters with targets has been the subject of recent experimental and theoretical activity [1–3]. In this paper we deal with the energy loss and disintegration of energetic C_{60} clusters in very thin Lindhard gas targets. Following Arista [5] particular emphasis is placed on the influence of the collective effects on stopping, brought about by the vicinage effect resulting from the proximity of the cluster ions to each other at the early stage of the Coulomb explosion. The dynamics of cluster breakup is followed in detail by means of a molecular-dynamics calculation, while the charge state, which is crucial in the molecular-dynamics calculation, is determined by the various processes of capture and loss of electrons.

In calculating the ionic charge state we neglect the very short early stage of the loss of molecular stability. It is assumed that the initial state of the projectile cluster is that of neutral carbon atoms at their original positions in the molecular cluster. Ionization of the individual carbon atoms is determined by the interaction of each of these with the plasma [4].

The forces driving the Coulomb explosion are taken as following from the screened Coulomb two-body potential V:

$$V=-\frac{e}{r}\exp(-r/a), \quad a=v_p/\omega_p .$$

Here r is the distance between two fragment ions, a is the screening length, v_p is the projectile velocity, and ω_p is the plasma frequency. The ionic motion that follows from these forces was calculated in the usual "leap-frog" algorithm used in molecular-dynamics simulations [6].

The energy loss of cluster ions was calculated by Arista [5], within the linear response approximation. Following his derivation, we use

$$\frac{dW}{dt}=-\sum_j \vec{v}\vec{F}_j=\frac{e^2}{2\pi^2}\int d^3k\,\frac{\vec{k}\cdot\vec{v}}{k^2}\mathrm{Im}\left(-\frac{1}{\epsilon(k,\vec{k},\cdot\vec{v})}\right)\times\left(\sum_i Z_i^2+\sum_{i\neq j} Z_iZ_j\cos(\vec{k}\cdot\vec{r}_{ij})\right). \quad (1)$$

Here $\vec{v}$ is the velocity (assumed to be common to all fragment ions), $\vec{k}$ is the wave vector upon which the integration is carried out, Z_i is the charge number of ion i, $\vec{r}_{ij}$ is the distance between ions i,j, and $\epsilon(k,w)$ is the Lindhard [7] dielectric function. The first term in large parentheses gives the energy loss of the individual independent charges. The second term gives the interference effect due to the charges in correlated motion. The assumption of velocity common to all ions in the cluster is justified in our case by the fact that during the short time in which the interference effect is important the differences that develop between individual velocities can be neglected.

The Lindhard dielectric function is described in detail by Lindhard and Winther [7]. This function is given in the (u,z) plane where z is proportional to k and u is given by ω/k. As a first step we locate the position in the (u,z) plane of the resonance line, which accounts for the collective effects. Next the resonance line is transformed to the (ω,k) plane, since the integration in Eq. (1) is carried out in these variables. $\mathrm{Im}(1/\epsilon)$ on the resonance curves is given by

$$\mathrm{Im}\left(\frac{1}{\epsilon}\right)_{\mathrm{res}}=\pi\left(\frac{\partial\mathrm{Re}(\epsilon)}{\partial\omega}\right)^{-1}\delta(\omega-\omega_{\mathrm{res}})=\pi\left(\frac{\partial\mathrm{Re}(\epsilon)}{\partial u}\frac{\partial u}{\partial\omega}\right)^{-1}\delta(\omega-\omega_{\mathrm{res}}).$$

This expression is inserted into Eq. (1), yielding the resonance contribution to the stopping that includes the vicinage effect. Stopping due to the collisional component is also calculated using Eq. (1), where the collisional part of $\mathrm{Im}(1/\epsilon)$ is considered.

Two basic types of calculations were carried out. "Static calculations" in which the total stopping power of a hypothetical C_{60} carbon cluster, consisting of 60 singly charged ions in the unperturbed C_{60} "fullerene" configuration, were calculated. These calculations were carried out as a function of cluster kinetic energy and also as a function of the density of the Lindhard gas. The other type of calculation involves the disintegration and stopping of a C_{60} cluster as it penetrates a foil of the Lindhard gas of density 10^{23} cm^{-3}, as discussed above. The background ions are assumed to be of charge 3, as in Al.

The results of "static calculations" as a function of the kinetic energy of the individual carbon constituent of the

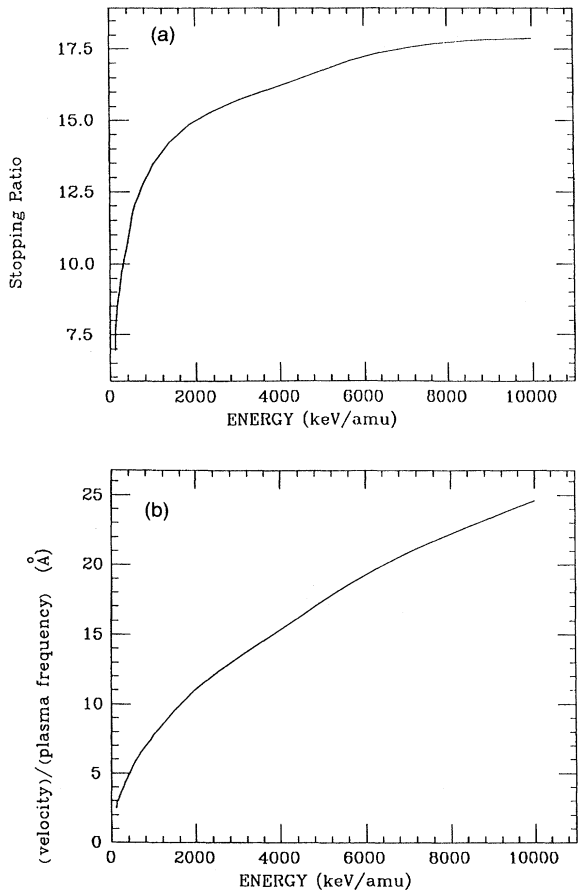

FIG. 1. (a) Stopping ratio, defined as the total C_{60} cluster stopping in the unperturbed "fullerene" configuration, divided by the sum of the stopping power of 60 individual carbon ions, as a function of kinetic energy. The density of the Lindhard gas is 10^{23} cm^{-3}. (b) Cluster velocity divided by plasma frequency, in angstroms, as a function of kinetic energy.

cluster are presented in Fig. 1(a). Here the stopping ratio is defined as the total C_{60} cluster stopping, including the vicinage effects, divided by the sum of the stopping power of 60 individual singly charged carbon ions. The electron density of the target is 10^{23} cm^{-3}. The contribution of the interference effects on the energy loss is seen to rise with energy, and the stopping ratio as defined above approaches a limiting value of about 19. By increasing the projectile velocity, the wake wavelength, which is proportional to v_p/ω_p, increases, and with this the domain of the interference or collective effects as well. In Fig. 1(b) is plotted v_p/ω_p as a function of the individual carbon energy. it is observed that when the length is close to 20 Å the stopping ratio begins to saturate. We note that the diameter of the C_{60} cluster is 7.08 Å, which is somewhat smaller than that.

"Static calculations" were also carried out as a function of the density, at the very high energy of 10 000 keV/A, where particular emphasis was placed on the stopping ratio due to the resonance stopping component. At a density of 10^{23} cm^{-3} this ratio is 40, while at 10^{21} cm^{-3} this ratio is 57.6. Thus at the lower density the cluster behaves essentially as a point charge, with charge 60, with respect to the stopping of the resonance component. As the plasma density decreases, the wake length v_p/ω_p increases with respect to the cluster dimensions, and at the density 10^{19} it is equal to 0.24×10^{-4} cm, much larger than the cluster diameter. The collisional contribution to the interference term is not accounted for in the above results. It was found that this effect is very small in comparison to the collective effects of the resonance contribution. The results for a C_{60} cluster at a kinetic energy of 200 keV/amu demonstrate this. Including the effect of interference on the collisional component of the stopping power gives an increase of 20% in the stopping powers of this component, which under these conditions is only 1.4% of the total stopping power.

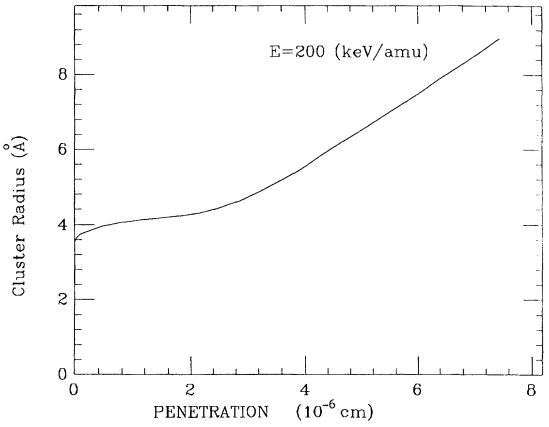

FIG. 2. Average C_{60} cluster radius as a function of the depth of penetration into a Lindhard gas of density 10^{23} cm^{-3}.

A dynamic calculation, including the disintegration and stopping of a C_{60} cluster of energy 200 keV/amu, was carried out for a Lindhard gas target at a density of $10^{23}e/cm^3$, which is 60% that of aluminum at normal solid density. The background charge of the target ions was assumed to be equal to 3. The calculation was carried out as described above and the average cluster radius as a function of penetra-

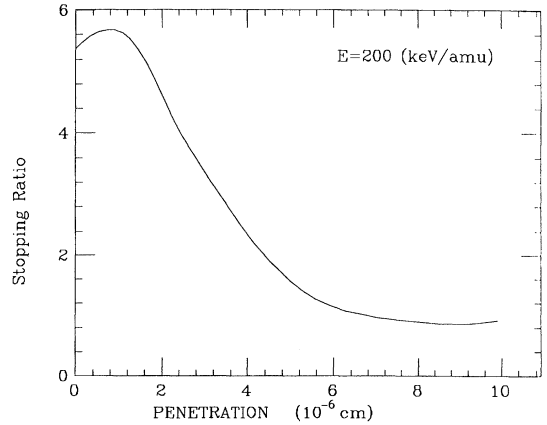

FIG. 3. "Stopping ratio," which gives the enhancement of the stopping power due to the vicinage effects, as a function of penetration for C_{60} at 200 keV/amu in a Lindhard gas of density 10^{23} cm^{-3}.

tion depth is plotted in Fig. 2. At depths greater than 4×10^{-6} cm the fragment motion is ballistic, indicating that the Coulomb interaction between the cluster constituents is screened out. Checking our projectile charge-state calculation we note that the dynamically calculated charge obtained here is 4.3, while the equilibrium charge is given by the "Betz curve" [8], with a slight extrapolation, is also 4.3.

The energy loss of the cluster as given in Eq. (1) is calculated at various distances of cluster penetration into the target. In calculating the energy loss, the directions of motion and energy of the cluster components are assumed to be the same as the initial values. These assumptions are justified in view of the low absolute energy loss and of the high ratio of longitudinal to transverse velocity. The charge states of each of the constituents are calculated independently of each other according to the discussion above. The "stopping ratio" as a function of the depth of penetration is given in Fig. 3. Upon entering the target, the energy deposition is enhanced by a factor of larger than 5. After penetrating 7×10^{-6} cm, the calculations yield no stopping enhancement; in fact, at this depth the stopping ratio falls a little below unity, indicating a negative contribution of the interference effects to the stopping.

The calculated total energy loss of a 2.4-MeV carbon atom penetrating a 0.1-μm-thick aluminum target is 0.133 MeV [9]. The bound-electron contribution to stopping in aluminum at this energy is only about 15% [10], thereby justifying the assumption that the aluminum target can be approximated by a Lindhard gas of the three free electrons. Assuming that the enhancement of the stopping power of a C_{60} cluster is that given in Fig. 3 (although the density in this figure is 60% that of the free-electron gas in aluminum), the average energy loss of a carbon atom originally in the incoming carbon cluster is 0.25 MeV. The difference of 0.12 MeV in the exit energy could be rather easily detected experimentally. The feasibility of similar experiments could be investigated for carbon, a material of which very thin targets could be fabricated.

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