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Energy loss of fast particles in confined atomic systems at very high temperatures

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Using a self-consistent description of an inhomogeneous electron gas in thermal equilibrium, we formulate a simple model for the stopping power of confined atomic systems at high temperatures. The model is based on previous studies of the energy loss of particles in partially degenerate plasmas. We describe the thermal enhancement of the energy loss in pellet fusion targets, in accord with recent experiments, and we explain this behavior in terms of quantum-mechanical and thermal effects in partially degenerate systems.

In the last years much interest has focused on the possibility of using light ion beams as drivers for inertial-confinement fusion (ICF).[1,2] This stems both from the property of efficient beam-target energy coupling and from the possibility of controlling and adjusting the energy deposition profiles. In this respect, ion-beam fusion has emerged as an important alternative in ICF studies.

Theoretical predictions[1,2] and experimental evidences[3,4] show the existence of a strong enhancement in the energy loss of proton and deuteron beams in heated solid targets as compared with the values in cold media. This effect has been theoretically explained[1,2] in terms of changes in the contributions of bound and free electrons in dense ionized media. The calculation of the energy loss by this approach requires evaluations of the degree of atomic ionization and average ionization potentials, or the use of approximate scaling laws, for a wide range of temperatures.

We present in this paper a simple and accurate model for calculating the energy loss of swift particles in solids at very high temperatures. The model is based on previous studies of dielectric response and stopping powers of dense plasmas at all degrees of degeneracy, and on a generalization of the Thomas-Fermi model for confined atomic systems at finite temperatures. Information of atomic structure parameters is not required in this approach. The treatment permits a complete analysis of the density and temperature dependences, and provides a novel explanation for the enhancement effect in the stopping power.

We base our description on previously derived analytical expressions for the stopping power of a dense electron plasma for all degrees of degeneracy.[5-8] From a dielectric treatment of elementary excitations in a dense plasma of density n and temperature T, the energy loss of a particle of charge $Z_1 e$ and velocity v, $S(n,v,T) \equiv -dE/dx$, can be cast in the usual form

$$S(n,v,T)=\frac{4\pi n Z_1^2 e^4}{mv^2}L(n,v,T) \;. \tag{1}$$

The "stopping number" L can be calculated analytically for the cases of low and high velocities; we quote here the results:

$$L(n,v,T)=\begin{cases} \dfrac{1}{2}\left[\dfrac{v}{v_F}\right]^3 \dfrac{\ln\Lambda(n,T)}{[1+\exp(-\mu/kT)]}, & v<v_c \quad \text{(2a)} \\[2ex] \ln\left[\dfrac{2mv^2}{\hbar\omega_P}\right]-\dfrac{\langle v_e^2\rangle}{v^2}, & v>v_c \quad \text{(2b)} \end{cases}$$

where ω_P is the plasma frequency, v_F is the Fermi velocity, μ is the chemical potential, k is Boltzmann's constant, and v_c is the velocity corresponding to the energy loss maximum (in practice v_c is taken as the velocity where the two expressions intersect). The low-velocity "collision logarithm," $\ln\Lambda$, is given by[8]

$$\ln\Lambda(n,T)=\ln(1+F)-F/(1+F) \;,$$

with

$$F(n,T)=\frac{16}{3}\left[\frac{E_F}{\hbar\omega_P}\right]^2+\frac{8}{\Gamma}\left[\frac{kT}{\hbar\omega_P}\right]^2 , \tag{3}$$

where E_F is the Fermi energy and $\Gamma=1.78$.

These expressions describe the temperature dependence of the energy loss. The high-velocity expression depends very weakly on temperature [the leading term in Eq. (2b) is independent of T]; therefore, the main temperature dependence arises in the low-velocity domain.

We now consider the description of electron density distributions in atomic systems under conditions of high pressures and temperatures. A generalization of the Thomas-Fermi model for atomic systems at finite temperatures was presented much earlier by Marshak and Bethe,[9] and it was studied in detail by Feynman *et al.*[10] and by Latter.[11] We use this approach to derive the electron density profiles for various atomic densities and temperatures.[12] To this end we consider an atom, with atomic number Z_2 and mass A, and we define a Wigner-Seitz sphere of radius r_0 (the value of r_0 is fixed by $4\pi r_0^3/3 = Am_P/\rho$, where ρ is the mass density of the solid). We must also apply the appropriate boundary conditions to confine the atomic system within this sphere.

With the assumption of spherical symmetry, we express the electron density $n(r)$, for a self-consistent potential $V(r)$, by integrating over a Fermi-Dirac distribution (for a partially degenerate plasma) as follows:

$$n(r) = \frac{1}{\pi^2\hbar^3}\int_0^\infty dp \frac{p^2}{1+\exp[\beta(p^2/2m - eV(r)) - \eta]}, \quad (4)$$

where $\beta = 1/kT$, p denotes the electron momentum, and η is a degeneracy parameter. Using Poisson's equation we obtain an integrodifferential equation for the potential $V(r)$, namely

$$\nabla^2 V(r) = \frac{2}{\pi\hbar^3}(2mkT)^{3/2} I_{1/2}(eV(r)/kT - \eta) \quad (5)$$

in terms of a Fermi integral $I_\nu(x)$ of order $\nu = \frac{1}{2}$.[13]

For a given density ρ and temperature T, Eq. (5) is solved by numerical integration, starting from the cell border, $r = r_0$, and with the boundary condition corresponding to a neutral system ($dV/dr = 0$ at $r = r_0$).

We show in Fig. 1 a set of results of electron density profiles for gold atoms at normal density, $\rho = 19.3$ g/cm^3, and for various temperatures. We observe that at these high temperatures, electrons are gradually removed from the ion core, and distributed in a more uniform way through the cell (in the limit $T \to \infty$ a uniform electron distribution with density $n = 0.686$ a.u. would be obtained).

Using this generalization of the Thomas-Fermi model we calculate the stopping power of a confined atomic system with temperature T and electron density $n(r)$, by integrating over the atomic cell, namely

$$\frac{dE}{dx} = \frac{4\pi Z_1^2 e^4}{mv^2}\int_0^{r_0} n(r) L(n(r), v, T) 4\pi r^2 dr, \quad (6)$$

where the density $n(r)$ is determined from Eqs. (4) and (5), and the stopping number L is calculated according to Eqs. (2a) and (2b) [the degeneracy of the electron gas varies with the local parameter $E_F(r)/kT$].

Figure 2 shows the energy and temperature dependence of the stopping power for protons in gold. The dashed line indicates available experimental results[14] for room temperature ($T = 0$); they are in good agreement with calculations above 200 keV.

We find also the following features: (a) With increasing temperature the maximum of the stopping power shifts to higher energies, and (b) the values near these maxima are larger than for cold targets (stopping enhancement).

For fixed energy, the temperature dependence of the stopping power always shows an enhancement followed by a decline. This is clearly seen in Fig. 3, where we show results for 1-MeV protons in Au for a series of densities, as a function of the target temperature. Calculations here extend to various densities ρ equal and smaller than the normal value, $\rho_0 = 19.3$ g/cm^3.

The maxima of the energy loss curves in Fig. 3 occur for $kT \cong 350$ eV, but the enhancement is stronger for lower densities. This range of densities and temperatures is the one of interest for studies of energy deposition profiles in the dense plasma corona that forms in heated ICF targets. We also note that the values calculated here are in agreement with the magnitude of the experimental observation of stopping power enhancements.[3,4]

Our model provides a physical explanation of this enhancement in terms of quantum and thermal effects in a partially degenerate electron gas. These effects are con-

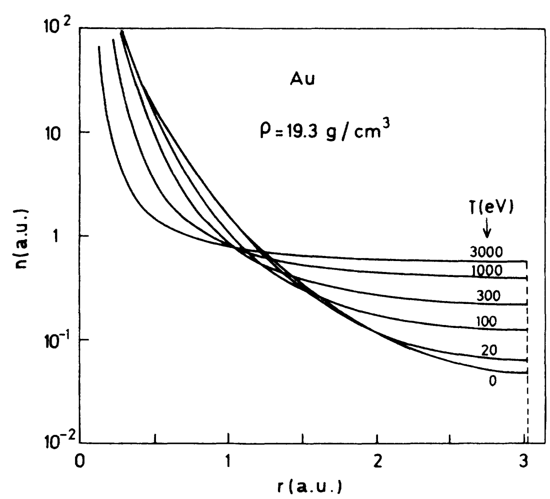

FIG. 1. Profiles of electron densities (in atomic units) for gold atoms confined within a spherical cell of radius $r_0 = 3.02$ a.u. (this corresponds to the normal density, $\rho = 19.3$ g/cm^3). Calculations are shown for temperatures $T = 0$, 20, 100, 300, 1000, and 3000 eV.

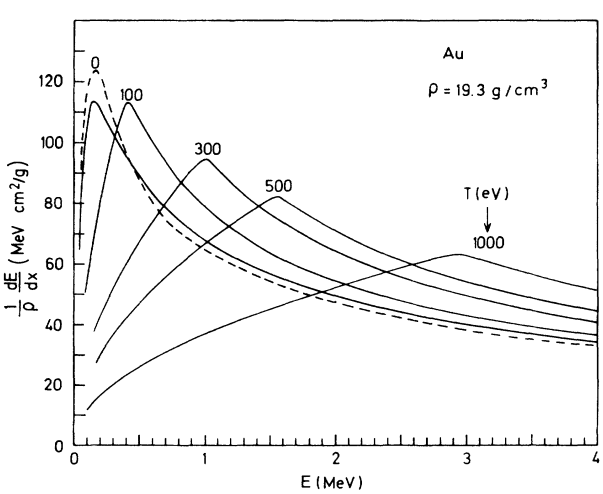

FIG. 2. Stopping power of confined gold atoms, according to the model described in the text, for temperatures $T = 0$, 100, 300, 500, and 1000 eV, versus proton energy. The dashed line indicates the experimental values for cold targets.

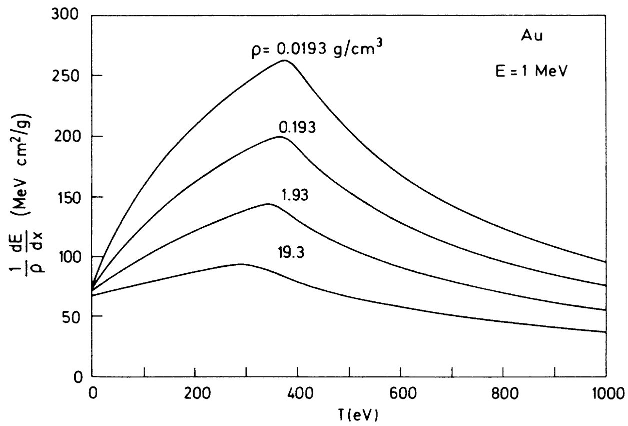

FIG. 3. Density and temperature dependence of the stopping power, for 1-MeV proton beams in gold. The enhancement of the energy loss becomes greater at lower densities, due to a larger relaxation of quantum constraints (see the text for discussion).

tained in Eqs. (2a) and (2b). As noted before, the main temperature dependence arises from the low-velocity expression. In particular, Eq. (2a) leads to the following limits (the values are given here in atomic units): (a) for $kT \ll E_F$,

$$S(n,v,0) \cong \frac{4Z_1^2}{3\pi} v \ln\left[\frac{4}{\sqrt{3}}\frac{E_F}{\omega_P}\right], \quad (7a)$$

and (b) for $kT \gg E_F$,

$$S(n,v,T) \cong \frac{4}{3}\frac{(2\pi)^{1/2}}{(kT)^{3/2}} Z_1^2 n v \left[\ln\left[\frac{kT}{\omega_P}\right] + \frac{1}{4}\right]. \quad (7b)$$

It can be shown that the departure of the leading linear density dependence in $S(n,v,0)$ [cf. Eq. (1)] is a direct consequence of the exclusion principle,[8,15] which gives place to the factor $(v/v_F)^3$ in Eq. (2a). This produces a strong reduction of the energy loss (in fact, the exclusion principle inhibits most of the transitions of those electrons inside the Fermi sphere, so that only electrons with velocities close to v_F can participate in the low-velocity range). For high temperatures, the factor v_F^3 is canceled out by the term

$$1+\exp(-\beta\mu) = \exp(\beta|\mu|) \propto (kT/E_F)^{3/2}$$

in Eq. (2a), and the "classical" dependence in $n/T^{3/2}$ is retrieved [note, however, that our result for the logarithmic term in Eq. (7b) is still quantum mechanical, as it should be in this case[16]].

To summarize these results in a convenient form, we define a "specific" stopping power (or stopping coefficient), $s \equiv S/n$, which represents the plasma stopping power "per electron." Then, we remark the following effects in a dense electron plasma: (a) an effect of "quantum transparency," with origin in the exclusion principle, leading to a decrease of $s \propto 1/v_F^3$ with increasing v_F; and (b) an additional effect of "classical (or thermal) transparency" which further reduces the energy loss; in particular, for $kT \gg E_F$ it leads to a dependence of the form $s \propto 1/T^{3/2}$.

To see how these effects give place to the energy loss enhancement shown in Fig. 3, we first note that the initial effect of the temperature arises through the modification of the density profile $n(r)$, in which electrons are removed from the high-density region of the core, and are distributed in the outer region of the atomic cell, with lower values of both local densities $n(r)$ and Fermi velocities $v_F(r) \propto n(r)^{1/3}$. Since the exclusion principle strongly inhibits excitations in the inner region of high densities, the local values of the specific stopping power are smaller in the atomic core than in the outer region. Hence, the enhancement of the energy loss can be attributed to a relaxation of the exclusion constraints, due to the spatial redistribution of electrons into regions of lower degeneracy [smaller $v_F(r)$].

At still higher temperatures, the effects of partial degeneracy become of increasing importance, and a distinct classical behavior arises. For $kT > E_F(r)$, the classical $T^{-3/2}$ dependence takes over, and produces the final decline of the stopping power, also illustrated in Fig. 3.

We can finally note that this explanation of the enhancement effect, which arises in a natural way from the description of the atomic electrons given by our model, is also consistent with the one given by previous authors[1,2] in terms of contributions from bound and free electrons (in particular, the redistribution of electrons can be regarded as ionization of the atomic core).

In conclusion, we present a new approach to calculate the energy loss of swift particle beams in confined atomic systems at very high temperatures. The model provides a unified description based on analytical results for partially degenerate plasmas (from dielectric response and energy loss studies), and on a generalization of the Thomas-Fermi model for confined atoms at finite temperatures. This permits a fast evaluation of the energy loss, through a self-consistent description of an electron gas of varying degeneracy, and does not require the determination of wave functions or atomic structure parameters. The model describes the enhancement effect in the energy loss of heated targets, as a result of a competition between quantum and thermal effects in partially degenerate systems.

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