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Electron Transport in Methane Gas

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We propose a kinetic theory for electron–drift-velocity maxima in polyatomic gases. The case of methane is considered in detail, and good agreement with experiment is obtained with use of model cross sections. The Boltzmann equation is solved directly by applying an iterative numerical technique, which converges well when inelastic scattering effects are important.

We consider the drift velocity V_d (average velocity) of a swarm of electrons in a steady determined by the action of a uniform electric field $\vec{E}$ and scattering from the molecules of a gas. For several polyatomic gases, V_d exhibits a maximum as a function of E.[1,2] It has been clear for a long time that inelastic scattering including a vibrational transition is involved (Cottrell and Walker[1]). However, no satisfactory kinetic theory has been presented to explain this feature. In this Letter, we give a general theory for it. We consider methane in particular, since it has been extensively studied from both an experimental and theoretical viewpoint[3] and its behavior is typical of several nonpolar polyatomic gases (e.g., CD_4, SiH_4, SiD_4, C_2H_4, C_2H_6). We propose that the velocity maximum is due to a strong "streaming" anisotropy in the electron velocity distribution $f(\vec{V})$. This results from the combined effects of elastic and inelastic scattering near the Ramsauer minimum in a way not previously understood in gas kinetic theory. To check our model quantitatively, we solve the appropriate Boltzmann equation for $f(\vec{V})$ for model scattering cross sections appropriate to methane. This is done by applying an iterative numerical technique originally developed by Rees[4] for what is essentially the same transport problem in semiconductors.

The iterative technique is numerically exact and converges well when $f(\vec{V})$ is anisotropic. Previous calculations of $f(\vec{V})$ in similar circumstances are all based on equations appropriate when anisotropy is small (see Huxley and Crompton[1] for a review of this work and references). Apparently the general condition for this is that the total inelastic cross section be much smaller than the total elastic cross section.[5] In the present model, this is not the case for most energies of interest [see Eq. (5)]. A strong anisotropy is also consistent with Cottrell and Walker's[1] demonstration that V_d is of the order of the rms electron speed for the fields considered here. Another consequence is that the elastic *energy loss* (and, in this context, the elastic momentum-transfer cross section) plays almost no role since it is far smaller than the inelastic energy loss. (The direction-changing effects of elastic scattering are crucial, however; see below.) Setting $m/M = 0$ in Eq. (2) at a typical value for E in the calculation described below affected only the fourth significant digit in $f(\vec{V})$.

It is worth emphasizing that the iterative technique[4] is very general and widely applicable to the problem of calculating $f(\vec{V})$ in similar electron- or ion-transport problems from given cross sections. It should prove especially useful

when the anisotropy of $f(\vec{V})$ is significant. This technique has apparently not previously come to the attention of workers concerned with swarm experiments in materials other than semiconductors.

The origin of the "streaming" anisotropy may be understood qualitatively as follows. For energies near the Ramsauer minimum (~0.3 eV in CH_4) the elastic cross section σ_{el} is small [see Eq. (5)]. In this energy range there is an inelastic process[6] that involves excitation of the first vibrational level. The threshold energy for this is 0.162 eV. Since this energy is well above kT for the relevant experiments and the electron density is low, we consider inelastic energy-loss collisions only (i.e., we neglect superelastic collisions). For small electric fields, most of the electrons will be at small velocities. In this region, the large elastic cross section produces large changes in the direction of motion of a given electron, but very small energy changes. An almost isotropic $f(\vec{V})$ (and small V_d) result. As $\vec{E}$ increases, more electrons are pulled in the $-\vec{E}$ direction, and attain energies in the Ramsauer-minimum region. If the effects of σ_{el} are sufficiently small there, most of them will be scattered inelastically back to velocities near $V=0$ rather than "spreading out" in velocity space. Thus, $f(\vec{V})$ will grow a "tail" in the direction opposite to $\vec{E}$.[7] With the model methane cross sections of Eq. (5), $f(\vec{V})$ has just such an anisotropy (see Figs. 2 and 3). As E increases further, the tail extends to larger V, where σ_{el} is large again. Electrons in this region contribute relatively less to V_d, since the larger elastic scattering makes $f(\vec{V})$ more isotropic. The ratio of $f(-V\hat{E})$ to $f(V\hat{E})$ at typical E values for the methane calculation described below indeed shows a maximum in the Ramsauer-minimum region (see Figs. 2 and 3).

The V_d maxima for the other molecules mentioned above may be explained similarly. There is evidence for a low-energy inelastic vibrational process for each of them.[8] A Ramsauer minimum may be expected in C_2H_6 since its total cross section is similar to CH_4 above 1 eV.[9] The total cross section for C_2H_4 is rising rapidly with energy at 1 eV.[10] A Ramsauer minimum has been assumed[11] for SiH_4. σ_{el} values for CD_4 and SiD_4 should be very close to those of CH_4 and SiH_4, respectively.

One can make a rough calculation of these effects for methane by assuming $f=$ const. for $V<V_c=24.4\times10^6$ cm/sec (the inelastic threshold), $\sigma_{in}\propto V^{-1}\theta(V-V_c)$, where θ is the unit step function, neglecting "in"-type inelastic scattering, and estimating the "direction-mixing" effects of σ_{el} for $V>V_c$. One finds that V_d rises approximately linearly with E. Fitting the slope to the experimental data gives a total inelastic cross section $\sigma_{in}{}^{tot}\cong1$ Å^2 (it is not surprising that the more accurate calculation mentioned below assumes a smaller value since we have neglected the shape of f for $V<V_c$). The condition on σ_{el} is more complicated. If we assume that its shape is similar to the σ_{el} of Eq. (5) and that the peak in V_d corresponds to a tail extending from $V=(30-50)\times10^6$ cm/sec, then the requirement that an electron traversing this region have a small probability of being elastically scattered gives $\sigma_{el}{}^{tot}\ll\sigma\simeq0.5$ Å^2 at the Ramsauer minimum.

To test this picture of the peak in V_d more completely we have solved the Boltzmann equation implied by the above discussion. This is

$$(eE/m)(\partial f/\partial V_z)=n\int V'S(\vec{V},\vec{V}')f(\vec{V}')d^3V'-nV\lambda(\vec{V})f(\vec{V});\quad \lambda(\vec{V})\equiv\int S(\vec{V}',\vec{V})d^3V', \tag{1}$$

where e and m are the electron charge and mass, n the number density of scatterers,

$$S(\vec{V},\vec{V}')=(V'^2/V^3)\sigma_{el}(V',\theta_S)\delta(V'-V[1+(m/M)(1-\cos\theta_S)])+(1/V)\sigma_{in}(V',\theta_S)\delta(V'-(V^2+V_c^2)^{1/2}), \tag{2}$$

σ_{el} and σ_{in} are the elastic and inelastic double-differential cross sections, respectively, and M is the scatterer mass. Following Rees[4] we convert Eq. (1) to an integral equation by adding $\Gamma f(\vec{V})$ to each side and treating the resulting right-hand side as an inhomogeneous term. One finds

$$\int K(\vec{V},\vec{V}')f(\vec{V}')d^3V'=f(\vec{V}), \tag{3}$$

where

$$K(\vec{V},\vec{V}')=\int_{-\infty}^{V_z}\exp[-\Gamma(V_z-V_z'')/E]n\{V'S(V_x,V_y,V_z'',\vec{V}')-[\Gamma-\lambda(\vec{V}')V']\delta^{(2)}(V_{xy}-V_{xy}')\delta(V_z''-V_z')\}(dV_z''/E). \tag{4}$$

Equation (3) may be solved by iterating the kernel K.[4] If $K\geq0$, and K is continuous except for jump

discontinuities, it has a unique positive eigenfunction corresponding to its largest eigenvalue.[12] In solving Eq. (3), Γ is varied to optimize the rate of convergence of the iteration.[4]

The only direct measurement of low-energy-electron cross sections in methane is apparently the total-cross-section work of Ramsauer and Kollath.[13] Values for the elastic momentum-transfer cross section and σ_{in} have been deduced from transport experiments.[3,11] However, these suffer the disadvantage of having been obtained by combining experiment with an approximate version of the Boltzmann equation which we believe requires some correction when $f(\vec{V})$ is strongly anisotropic. The only calculation of σ_{in} that we are aware of is the Born-approximation work of Davis and Schmidt.[6] Their σ_{in} agrees in shape with that deduced from transport data[11] but is about a factor of 3 smaller. This disagreement may be due to the inadequacy of the Born approximation, the approximate kinetic-theoretical treatment of the transport data, or the presence of resonant effects (Boness *et al.*[6]). There seems to be only one calculation of σ_{el} (Gianturco and Thompson[3]) for which complete numerical results have not yet appeared.[14] Therefore, to demonstrate the quantitative validity of our explanation of the peak in V_d for methane, we used the model s-wave cross sections

$$4\pi\sigma_{el} = \begin{cases} 230(V^{-2} - 1/900) + 0.2, & V < 30, \\ 0.2, & 30 < V < 50, \\ (V - 50)/6 + 0.2, & V > 50, \end{cases}$$
$$4\pi\sigma_{in} = 0.63\,\theta(V - 24.4), \qquad (5)$$

where V is given in unity of 10^6 cm/sec, and σ in Å^2. The shape of the total cross section is similar to experiment.[13] σ_{in} is similar in shape and magnitude to that deduced by Pollock[11] (his value is about 0.8 Å^2) Using Eq. (5) and Ree's method[4] we obtained convergence of up to eight significant digits after 200 iterations. The eigenvalues were between 0.98 and 1. Our results for V_d are compared with experiment in Fig. 1. Error was estimated by varying the size of the region in which Eq. (3) was solved. Calculations done with s-wave σ_{el} values more than two times those of Eq. (5) and various shapes consistently produced V_d values smaller than those reported in Fig. 1, and V_d-vs-E curves that rose monotonically in most cases.

The cross sections assumed in Eq. (5) do not include any parametrization of the resonant effects known to exist above 1.75 eV (Boness *et al.*[6]). In this region σ_{el} is large, so that $f(\vec{V})$ will be isotropic and the main effect of σ_{in} will be to determine how $f(\vec{V})$ goes to zero as V increases This will depend on an appropriate average of σ_{in} over energy. Thus the V_d-vs-E curve will not be sensitive to the detailed shape of the cross sections outside of the Ramsauer-minimum region. Since the observed total cross section[13] is smooth in this region, we represent σ_{in} by a constant. (Including resonant effects in σ_{in} might improve the agreement of V_d with experiment at the larger E values considered, but this would be difficult to establish without a better model for σ_{el}.)

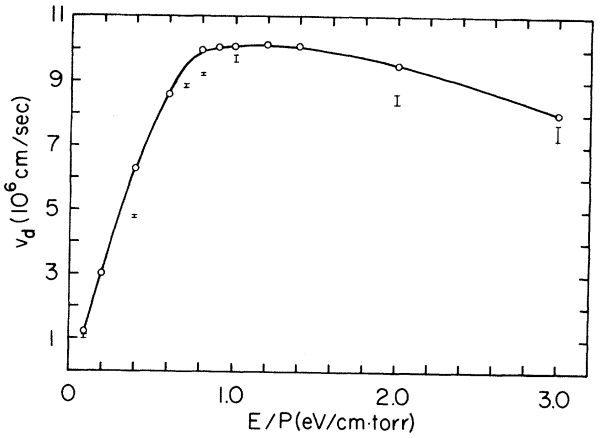

FIG. 1. Drift velocity V_d for electrons in methane gas at 293°K as a function of electric field E. Curve with circles, experimental values [from Pollock (Ref. 11) Fig. 1]; bars, present calculation. The vertical spread indicates estimated error.

The minimum total cross section from Eq. (5) is 0.83 Å^2. Experiment puts this quantity at 1.4 Å^2.[13] This discrepancy is likely due to the assumption that σ_{el} is isotropic. A cross section peaked in the forward direction would be much less effective in reducing the anisotropy in $f(\vec{V})$. If one takes the step length in a random walk proportional to the angular width of σ_{el}, the number of steps in a given time is proportional to the total elastic cross section. Then simple arguments show that the rms angular deviation for the (s-wave) σ_{el} of Eq. (5) is the same as that of a forward-peaked σ_{el} of width about 90° corresponding to a total elastic cross section of 0.77 Å^2. With this σ_{el} the total cross section agrees with experiment. An even greater narrowing of σ_{el} has been observed near the Ramsauer minimum in Kr and Xe.[15]

A plot of $f(\vec{V})$ for two field values of E is given in Figs. 2 and 3. The qualitative behavior dis-

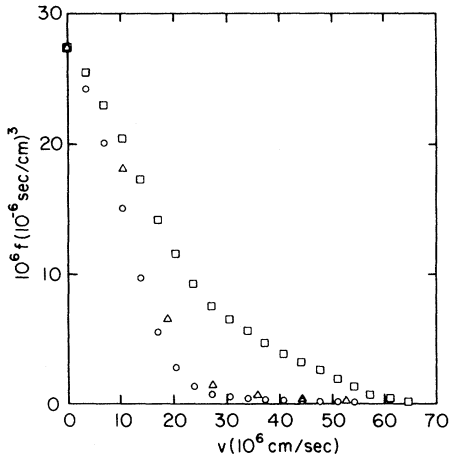

FIG. 2. Normalized velocity distribution function for $E/p = 0.8$ eV/cm Torr. The upper curve (squares) is in the $-\vec{E}$ direction, lower curve (circles) in the $\vec{E}$ direction, and middle curve (triangles) perpendicular to $\vec{E}$.

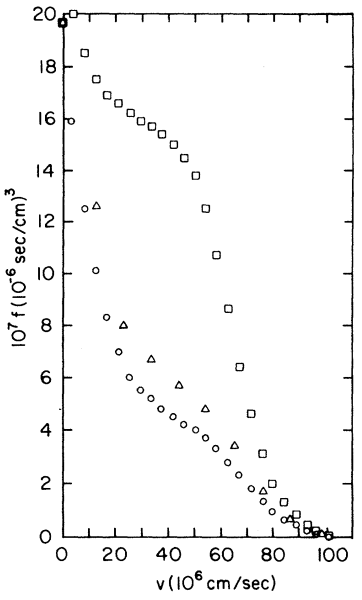

FIG. 3. Normalized velocity distribution function for $E/p = 3.0$ eV/cm Torr. Symbols have the same significance as in Fig. 2.

cussed above is apparent

We believe the results for methane reported here demonstrate the validity of the kinetic-theoretical ideas proposed and also the efficacy of direct solution of the Boltzmann equation. More elaborate computational efforts (e.g., including the energy dependence of the angular width of σ_{el} and more detailed modeling of σ_{in} to include resonances, higher excited states, and angular dependence) should be strongly coupled to better characterization of the cross sections since transport data cannot uniquely determine σ_{el} and σ_{in}.

We would like to thank Dr. R. N. Silver for pointing out the trail leading to Rees's method (Ref. 4), Dr. M. Feinstein for bringing the article by Gianturco and Thompson (Ref. 3) to our attention, and Professor D. G. Truhlar for helpful comments on the manuscript. This work was supported in part by grants from the National Science Foundation and the American Chemical Society–Petroleum Research Fund.

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Drift-Modified Tearing Instabilities Due to Trapped Electrons

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It is shown that the collisional detrapping of magnetically trapped electrons in tokamaks can excite drift tearing modes with high azimuthal mode numbers. For normal temperature gradients ($d\ln T_e/d\ln n > 0$), the modes are unstable in the collisional regime ($\nu_{\rm eff} > \omega_{*e}$), but stable in the collisionless regime ($\nu_{\rm eff} < \omega_{*e}$).

The parameters of present and future generations of tokamaks lie in the trapped-electron regime, in which the trapped-electron bounce frequency exceeds the effective collision frequency. Electrostatic microinstabilities of the drift-wave type (in particular, trapped-electron modes[1]), which are driven unstable by the expansion free energy associated with the density and temperature gradients, have been studied in some detail, because of their possible contribution to the anomalous cross-field transport processes. In this Letter, we show that the same free energy can also drive a tearing[2] or, more precisely, a drift-modified tearing instability.[3] In contrast to the finite-β modified trapped-electron instability,[4] these modes connect to long-wavelength magnetohydrodynamic (MHD) perturbations, rather than propagating sound waves, away from the mode rational surfaces. This new instability, which we call the dissipative trapped-electron drift tearing mode, will cause the formation of magnetic islands. In this way, the new instability could have a significant effect on cross-field transport, by mechanism different from those involving only *electrostatic* trapped-electron modes.

The wave equation for this mode is derived following fairly standard procedures.[4] For tokamaks with $\beta \equiv 8\pi p/B^2 \lesssim \epsilon/q^2 \ll 1$, the compressional Alfvén wave can be ignored, and the perturbed magnetic vector potential is given by $\vec{A} = A_\parallel \vec{B}/B$. Here, $\epsilon = r/R$, and $q = rB_T/RB_P$ is the safety factor. The other perturbation-field quantity is the electric potential φ. We then have $\vec{E} = -\nabla\varphi - \partial\vec{A}/c\partial t$ and $\vec{b} = \nabla\times\vec{A}$.

The perturbed electron distribution function is determined by the drift kinetic equation:

$$f_e = e\varphi f_{e0}/T_e + h_e, \tag{1}$$

$$(\omega - \omega_D - iC + iv_\parallel\nabla_\parallel)h_e = -\frac{ef_{e0}}{T_e}(\omega - \omega_*{}^T)\frac{\varphi - v_\parallel A_\parallel}{c}. \tag{2}$$

Here $\omega_*{}^T = \omega_{*e}[1 - \eta_e(\frac{3}{2} - \bar{v}^2)]$, $\bar{v} = v/v_{Te}$, $v_{Te} = (2T_e/m_e)^{1/2}$, $\eta_e = d\ln T_e/d\ln n$, ω_* is the electron diamagnetic drift, and ω_D is the combined electron ∇B and curvature drift. For the collision operator C, we assume a number-conserving, velocity-dependent Krook model; in this model, number conservation is satisfied by including in the equation for the untrapped electrons a Maxwellian source term equal to the number of electrons scattered out of the trapped region. For trapped electrons, Eq. (2) then gives

$$h_e{}^t = -\frac{ef_{e0}}{T_e}\frac{(\omega - \omega_*{}^T)A_\parallel}{ck_\parallel} + \hat{h}_e{}^t; \tag{3}$$

$$\hat{h}_e{}^t = -\frac{ef_{e0}}{T_e}\frac{\omega - \omega_*{}^T}{\omega - \langle\omega_D\rangle + i\nu_e(v)}\left(\varphi - \frac{\omega A_\parallel}{ck_\parallel}\right). \tag{4}$$

In Eq. (4), and in the following analysis, we neglect terms of order ω_D/ω; we keep ω_D only in denominators such as the one in Eq. (4), where it can give rise to resonance contributions, especially at small ν_e. For untrapped electrons, we obtain

$$h_e{}^u = -\frac{ef_{e0}}{T_e}\frac{\omega - \omega_*{}^T}{\omega - k_\parallel v_\parallel}\left(\varphi - \frac{v_\parallel A_\parallel}{c}\right) + \frac{if_{e0}}{\omega - k_\parallel v_\parallel}\frac{\int_t \nu_e(v)\hat{h}_e{}^t d^3v}{n_0[1 - (2\epsilon)^{1/2}]}. \tag{5}$$