Angular Dependence of Surface Scattering and Surface Mobility Cusp

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Recent theories of the surface mobility of semiconductors predict the existence of a cusp in the surface mobility as a function of surface-potential excess, if the surface is strongly scattering, and if the bulk mean free path is larger than the Debye screening length. Recent experiments on InSb surfaces, however, show no cusp. This disagreement is resolved by including an angular dependence in the Fuchs' reflectivity parameter p, which describes the surface scattering. It is concluded that: (a) a surface mobility cusp should occur if and only if electrons incident at grazing angles are strongly scattered, (b) observation of the existence or nonexistence of a surface mobility cusp on a particular surface provides insight into the scattering mechanisms dominant on the surface.

I. INTRODUCTION

SURFACE transport theory[1] has predicted that a semiconductor with a diffusely scattering surface should have a surface mobility with a cuspid dependence on surface-potential excess. The cusp should be significant in the nonlocal case[2]: viz., bulk mean free path λ_B greater than Debye screening length L. But, careful observations of Davis[3] on various InSb surfaces at 77°K, having $\lambda_B/L>2$, showed no cusp. Theory and experiment thus disagreed.

The theory was based on the space-dependent Boltzmann equation together with the well-known Fuchs' boundary condition (b.c.)[4] on the distribution function f_1:

$$f_1(v_x,v_y,v_z>0)=pf_1(x_x,\,v_y,\,v_z)\quad \text{at the surface, } z=0+\,, \tag{1}$$

where p is the Fuchs' reflectivity, a phenomenological constant.

Recently it has become clear that some generalizations of the Fuchs' b.c. are necessary: Aubrey, James, and Parrott[5,6] have shown that size effects in bismuth at 4.2°K can be understood only by permitting p to depend strongly upon the angle of the incident k vector. Greene has examined a number of surface-scattering mechanisms (surface electron-phonon coupling,[7] localized charged surface states,[8] Rayleigh waves[9]) and shown that p often depends strongly upon the angle and magnitude of the incident k vector. Also, Greene has shown[10] that a new b.c., differing significantly from Fuchs' b.c. in some respects, may be derived from first principles, and that p may be expressed in terms of the simplest properties of wave functions near crystal surfaces.

In this light we now show that the angular dependence of p is crucial for the existence of a surface mobility cusp: If the surface-scattering mechanism is ineffective for grazing angles of incidence, the cusp is absent; otherwise it should occur. This reconciles theory with Davis experiments[3] on InSb surfaces, and permits some inferences to be made about the scattering mechanism on those surfaces.

II. QUALITATIVE CONSIDERATIONS

It has been pointed out[2] that there is a number ΔN_1 of electrons, already present near the surface when the bands are flat, whose drift velocity is wiped out by turning on a small attractive surface potential if the surface is diffusely scattering. ΔN_1 comprises, when $\lambda_B/L\gg1$, all those electrons which are moving toward the surface $z=0$ with $mv_z^2/2kT<\Delta u(z)$, where $\Delta u(z)$ (kT/e) is the electrostatic potential at z relative to the bulk. The contribution of ΔN_1 to the surface conductance $\Delta\sigma$, and to the surface mobility μ_S $-e\mu_B\Delta N_1$, and $-\mu_B\Delta N_1/\Delta N$, respectively, where $\Delta N=\int dz(n-n_B)$ is the number of excess carriers and μ_B is the bulk mobility. Now $\Delta N_1\sim(2/\sqrt{\pi})n_BL\Delta_S u^{1/2}$ and $\Delta N=n_BL\Delta_S u$ for $0<\Delta_S u\ll1$, so that μ_S is singular at $\Delta_S u=0$. The singularity would be weaker, clearly, for smaller λ_B/L.

Now, instead of the completely diffuse surface, $p=0$, assumed above, let us assume that electrons are specularly reflected when their incident k vectors make large angles with the normal. We make a simple assumption about the form of p, similar to that made by Parrott[5,6];

$$p=1 \quad\text{for}\quad v_{\text{II}}^2/v_z^2>t^2\,, \tag{2a}$$
$$p=0 \quad\text{for}\quad v_{\text{II}}^2/v_z^2\le t^2\,, \tag{2b}$$
$$0<t^2<\infty\,,$$

where $v_{\text{II}}^2=v_x^2+v_y^2$. The number of electrons whose drift velocity is wiped out, when $\Delta_S u\ll1$ is turned on,

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[10] R. F. Greene, preceding article, Phys. Rev. **141**, 687 (1966).

by surface scattering is now no longer ΔN_1, but only

$$\Delta N_t=\int_0^\infty dz\int_{-v_{z0}}^0 dv_z\int_0^{2\pi} d\Phi\int_0^{tv_z} v_{\shortparallel}dv_{\shortparallel}n_B \times\left(\frac{m}{2\pi kT}\right)^{3/2}\exp\left(\frac{-mv^2}{2kT}-\Delta u\right), \quad (3a)$$

where

$$mv_{z0}^2/2kT-\Delta u(z)=0. \quad (3b)$$

One finds that

$$\Delta N_t\doteq(3/2\sqrt{\pi})n_BLt^2(\Delta_S u)^{3/2} \quad \text{for} \quad t^2\Delta_S u\ll 1. \quad (4)$$

The contribution of ΔN_1 to μ_S is now negligible compared to that of ΔN. We, therefore, expect no cusp when λ_B/L is finite, and grazing electrons are specularly reflected rather than scattered.

If the surface-scattering mechanism behaves in the opposite fashion, with grazing electrons scattered, and $p=0$ and $p=1$ interchanged in (2), then a cusp again occurs in μ_S. For now the number of electrons, whose drift mobility is wiped out by surface scattering when a small attractive surface potential is turned on, is $\Delta N_1-\Delta N_t\sim\Delta N_1$.

From these simple considerations it is apparent that the angular dependence of surface scattering is crucial to the existence of the surface mobility cusp.

III. QUANTITATIVE TREAMTENT

In the previous section we gave a simple heuristic treatment of the cusp for the limiting case of $\lambda_B/L\gg 1$. Here, we give a general Boltzmann equation treatment which, while less perspicuous, is both quantitative and valid for any value of λ_B/L.

Direct examination shows that Eqs. (3.4) of Ref. 1 (hereafter called GFZ) are valid for arbitrary angular dependence of $p(v_z^2,v^2)$. One finds

$$\frac{\mu_S}{\mu_B}=1-\frac{n_B\bar{\lambda}}{\Delta N}\left\{1-\int dv\int dv_z\int_0^\infty d\epsilon_{\shortparallel}\epsilon_{\shortparallel} \times e^{-\nu-\epsilon_{\shortparallel}}\left(\frac{h_p\lambda_B}{\bar{\lambda}}\right)\left(-\frac{\partial K}{\partial v_z}\right)\right\}, \quad \Delta_S u\geq 0 \quad (5a)$$

$$\frac{\mu_S}{\mu_B}=1+\frac{n_B\lambda}{\Delta N}\left\{1+\int dv\int dv_z\int^\infty d\epsilon_{\shortparallel}\epsilon_{\shortparallel} \times e^{-\nu-\epsilon_{\shortparallel}}\left(\frac{h_p\lambda_B}{\bar{\lambda}}\right)\left(-\frac{\partial K}{\partial v_z}\right)\right\}, \quad \Delta_S u\leq 0, \quad (5b)$$

where ν and v_z are integrated over the shaded portions of Fig. 1 of GFZ,

$$\bar{\lambda}\equiv\lambda_B\int_0^\infty d\epsilon_z\int_0^\infty d\epsilon_{\shortparallel}\epsilon_{\shortparallel}(1-p)\exp(-\epsilon_z-\epsilon_{\shortparallel}), \quad (5c)$$

$$\epsilon_z=mv_z^2/2kT, \quad \epsilon_{\shortparallel}=mv_{\shortparallel}^2/2kT,$$

K and ν are as in GFZ, (5d)

and

$$h_p=(1-p)\exp K(v_z,v_S)/[1-p\exp 2K(v_{zS},0)]. \quad (5e)$$

We again choose, for simplicity, the form (2) for p, so that the $\epsilon_{\shortparallel}$ integration becomes simple. We find

$$\frac{\mu_s}{\mu_B}=1-\left(\frac{n_B\bar{\lambda}}{\Delta N}\right)\left\{e^{\Delta_s u}-1 -\int_{-\Delta_S u}^0 d\nu\left(\frac{\lambda_B g_s}{\bar{\lambda}}\right)e^{-\nu-2K}\right\}, \quad \Delta_S u\geq 0 \quad (6a)$$

$$\mu_S/\mu_B=1-(n_B\bar{\lambda}/\Delta N)\{e^{\Delta_S u}-1\}, \quad \Delta_S u\leq 0, \quad (6b)$$

where

$$\bar{\lambda}/\lambda_B=t^4/(1+t^2)^2\leq 1 \quad (6c)$$

and where we put $\Delta u\sim\Delta_S u$ in

$$g_s=1-(1+t^2(\Delta_S u+\nu))\exp(-t^2(\Delta_S u+u)). \quad (6d)$$

We note that (6) reduces to the diffuse GFZ result when $t^2\to\infty$, in which case $g_s\to 1$, and the stagnation layer thickness[1] $\bar{\lambda}\to\lambda_B$.

Clearly a cusp exists when and only when the integral in (6a) has a finite (+) slope at $\Delta_s u=0+$. After some manipulation, we find (a) for $t^2=\infty$ (GFZ, diffuse)

$$\mu_S/\mu_B \xrightarrow[\Delta_s u\to 0+]{} 1-(\lambda_B/L)(1+\tfrac{1}{3}\Delta_S u) +(\tfrac{1}{2}\pi)(\lambda_B/L)^3\Delta_S u, \quad (7a)$$

$$\mu_S/\mu_B \xrightarrow[\Delta_s u\to 0-]{} 1-(\lambda_B/L)(1+\tfrac{1}{3}\Delta_S u); \quad (7b)$$

(b) for t^2 finite (grazing electrons specularly reflected)

$$\mu_S/\mu_B \xrightarrow[t^2\Delta_s u\to 0+]{} 1-(\bar{\lambda}/L)(1+\tfrac{1}{3}\Delta_S u) +(15\pi^3/8)(\lambda_B/L)^4t^4(\Delta_S u)^5, \quad (8a)$$

$$\mu_S/\mu_B \xrightarrow[t^2\Delta_s u\to 0-]{} 1-(\bar{\lambda}/L)(1+\tfrac{1}{3}\Delta_S u). \quad (8b)$$

Thus a cusp occurs when the surface is diffuse for all incident angles, but not when grazing electrons are specularly reflected. It can also be shown that when it is the normally incident electrons only which are specularly reflected [interchanging $p=0$ and $p=1$ in (2)], a cusp occurs.

IV. CONCLUSIONS

We have shown that the existence of a surface mobility cusp hinges upon the angular dependence of the Fuchs' reflectivity parameter p. A cusp is predicted when the surface scattering is effective for grazing angles, but not when grazing electrons are specularly reflected. This explains the absence of a cusp for the InSb surfaces studied by Davis,[3] provided we infer that these surfaces have scattering mechanisms which are ineffective for grazing electrons. Such an inference, although necessarily provisional in the absence of a treatment of the energy dependence of p, is interesting, inasmuch, as it agrees with the conclusion reached by Aubrey *et al.*[5] and Parrott[6] for the semimetal Bi at 4.2°K.

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Decay of Laser-Induced Excitations of *F* Centers*

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A strong population of excited F-center states is achieved in various alkali halides using a short intense pulse of a Q-switched ruby laser. During the presence of the excited F centers the time dependence of their decay is measured with a fast-recording spectrometer. This is done by monitoring the absorption changes connected with the ground-state or excited-state populations. Using this method for crystals containing low F-center concentrations, the lifetime of the excited state of F centers in KI, RbI, CsI, RbBr, and CsF is measured from 7 to about 80°K by monitoring absorption changes in the region of the β, the β^* and the F band, respectively. For KI samples containing high F-center concentrations it is found that the decay curves are nonexponential.

I. INTRODUCTION

THE knowledge of the lifetime of excited states is important for the understanding of the character of electronic transitions in solids. Allowed electric dipole transitions are expected to have lifetimes of the order of 10^{-8} sec. Recently, however, Swank and Brown[1] found for the excited state of F centers in some alkali halides lifetimes of the order of 10^{-6} sec. These results were rather surprising in view of the high absorption cross section of the F transition, and they stimulated a variety of theoretical considerations[2] on the nature of this excited state. A number of alkali halides have since been studied[3] by conventional techniques: After flash excitation of the F center by a very short light pulse the resultant decay of luminescence or photoconductivity was determined. Photoconductivity measurements were limited, however, to a temperature region where a sufficient concentration of electrons is still thermally stimulated into the conduction band from the excited state F^* of the F center. The lowest temperatures reached where about 70°K (F centers in KI, KBr, RbBr, and CsBr).[1,3] Luminescence measurements, on the other hand, were limited by the availability of fast detectors in the infrared region to F centers in KCl, NaCl, and RbCl.[1,3]

This paper reports measurements of the radiative lifetime of F centers in several alkali halides extending the range of observations to lower temperatures (in KI and RbBr) and other crystals (RbI, CsI, and CsF). The method is novel in that it employs a very intense, short light pulse from a Q-switched ruby laser, which in contrast to conventional methods pumps an appreciable number of the F centers in the specimen into the excited state. These changes of population of the ground state and the excited state are so large that transmission changes of the sample can now be directly observed with a fast-recording spectrometer. Because these changes occur in *any* of the various absorption bands connected with the ground or excited state of the F center, the time dependence of these population changes can be studied in various regions of the visible and near uv. The monitoring light source of the spectrometer, a xenon flash lamp, can be made sufficiently intense so that a rather good signal-to-noise ratio is achieved. In addition changes of population of the ground state and the excited state can be monitored independently. The method could therefore be used to check upon the exponential nature of the decay of population changes. For higher F concentrations in KI nonexponential decay curves were indeed observed.

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