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Analytical determination of the density-of-gap-states distribution in amorphous semiconductors

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We report on the analytical solution of the Fredholm integral equation of the first kind which relates the induced space-charge density, $\rho(V)$, to the density of gap states, $N(E)$. The formula for $N(E)$ is given for the general case in which $\rho(V)$ can be expressed as a polynomial function of the band-bending potential V.

The knowledge of the density-of-states (DOS) distribution in the energy gap of a semiconductor is a fundamental problem for the determination of its electronic properties. Up to now, many techniques have been used to determine the density of states. Unfortunately, each of them presents the same limitations[1] and, generally, the predictions of one technique do not coincide with those of another one. One of the more used techniques is the field-effect technique which allows one to measure the induced change in conductance of the semiconductor when an external voltage V_F produces a bending of the mobility edges of the valence and conduction bands upwards or downwards for negative or positive values of V_F, respectively. The bending is due to an electrostatic potential $V(x)$ which obeys Poisson's equation. The potential distribution in the space-charge region depends on the density-of-states distribution, $N(E)$, in the energy gap.

Lately, the method of calculation of $N(E)$ has been improved;[2-4] the calculation is based either on an iterative self-consistent method[2,3] or on a deconvolution procedure.[4] Both methods have several limitations. The iterative method does not allow one to decide about fine structures in the density-of-states curve,[2] while the deconvolution procedure[4] leads to a set of algebraic equations whose solution is, generally, physically unreasonable.[5]

In this note, we obtain a formal analytical solution of the Fredholm integral equation of the first kind which relates the density of the space charge $\rho(V)$ to the density of states $N(E)$:

$$\rho(V) = -e\int_{-\infty}^{+\infty} N(E)[f(E-eV)-f(E)]\,dE \ , \quad (1)$$

where $f(E)$ is the Fermi function, e the electronic charge, and V the potential inside the semiconductor.

By putting

$$y=\exp(eV/kT), \quad a=\exp(-E_f/kT) \ , \quad (2)$$

and introducing the variable

$$z=\exp(E/kT) \ , \quad (3)$$

Eq. (1) can be written as

$$\rho(V) = -e\int_0^{\infty} \frac{(y-1)\omega(z)}{y+az}\,dz \ , \quad (4)$$

where $V=(kT/e)\ln y$ and

$$\omega(z) = akTN(kT\ln z)/(az+1) \ . \quad (5)$$

It can be easily shown that Eq. (4) is the Stieltjes integral equation

$$(a/e)(1-ax')^{-1}\rho(kT\ln(ax')/e) = \int_0^{\infty} \frac{\omega(z)}{x'+z}\,dz \equiv \phi(z) \ , \quad (6)$$

where

$$x'=y/a \ . \quad (7)$$

Therefore, the problem of solving the Fredholm integral equation is reduced to that of solving the Stieltjes equation and determining, when it exists, the inverse Stieltjes transform, $\omega(z)$. To this aim, for the reader's convenience, we recall some properties of the Stieltjes transform (see, for example, Ref. 6).

First, the Stieltjes transform is connected to the Laplace transform in a simple way. In fact, if

$$\phi(s) = \int_0^{\infty} e^{-st}\Omega(t)\,dt \ , \quad (8)$$

where

$$\Omega(t) = \int_0^{\infty} e^{-tz}\omega(z)\,dz \quad (9)$$

we get formally

$$\phi(s) = \int_0^{\infty} \frac{\omega(z)}{s+z}\,dz \ . \quad (10)$$

Second, we have that if the integral (10) converges for a point $s=z_0$ not on the negative real axis, then it converges for every such point. Furthermore, (i) it converges uniformly in any closed bounded region not containing a point of the negative real axis, and (ii) it represents an analytical single-valued function in the complex-s plane cut along the negative real axis. We notice that our problem is reduced to finding an inversion formula for Eq. (8).

In order to illustrate the procedure of solution of Eq. (6), we limit ourselves here to providing an explicit example. In doing so, let us assume that the space-charge density is a polynomial function of the potential V:

$$\rho(V) = a_1V + a_2V^2 + \cdots + a_nV^n \ . \quad (11)$$

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It must be noted that in Eq. (11) the zeroth order term is missing; this has both physical and mathematical reasons. From Eq. (1), if $V=0$, $\rho(V)=0$, which occurs in flat-band conditions. On the other hand, the inverse Stieltjes transform does not exist if $\rho(V)$ is a constant. Moreover, this seems to exclude the possibility that the potential distribution inside the semiconductor has a parabolic profile, unless the density-of-states distribution in the energy gap is null.

Inserting Eq. (11) in Eq. (6) and taking account of Eq. (2), we obtain

$$\phi(x')\equiv\phi(y/a)=\frac{a}{e}\frac{1}{1-y}\rho\left(\frac{kT}{e}\ln y\right)$$
$$\equiv\frac{a}{e}\frac{1}{1-y}\sum_{m=1}^{n}A_m\ln^m y\ , \qquad (12)$$

where

$$A_m=a_m\left(\frac{kT}{e}\right)^m \quad (m=1,2,\ldots,n)\ . \qquad (13)$$

Now, let us consider the integral

$$\frac{1}{2\pi i}\oint_\Gamma e^{st}\frac{\ln^m s}{1-s}ds\ , \qquad (14)$$

where s is a complex variable and Γ is the contour of Fig. 1, where CBA and FED are arcs of a circle of radius R whose center is the origin 0, and GHI is the arc of a circle of radius ϵ (also with center at 0). Since the function $\ln^m s/(1-s)$ is analytic inside Γ and the integrals around the arcs CBA, FED, and GHI vanish as $R\to\infty$ and $\epsilon\to 0$, respectively, we are led to the expression

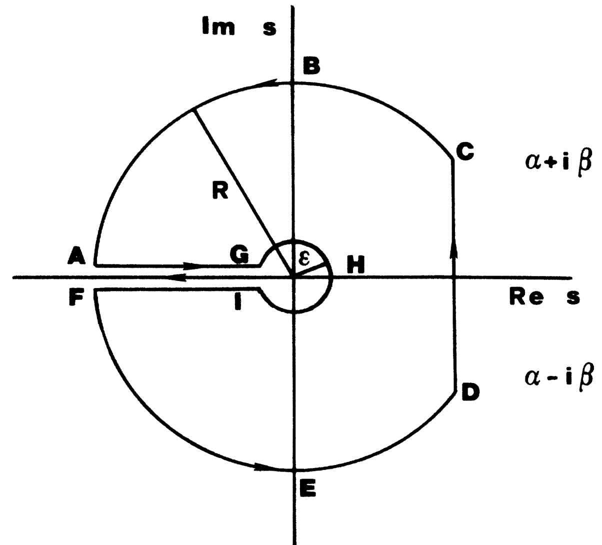

FIG. 1. Contour of integration of integral (14).

$$\lim_{\substack{R\to\infty\\ \epsilon\to 0}}\frac{1}{2\pi i}\oint_\Gamma e^{st}\frac{\ln^m s}{1-s}ds=\frac{1}{2\pi i}\left[\int_{\alpha-i\infty}^{\alpha+i\infty}\frac{e^{st}\ln^m s}{1-s}ds+\int_{-\infty}^{0}\frac{e^{xt}(\ln|x|+i\pi)^m}{1-x}dx+\int_{0}^{-\infty}\frac{e^{xt}(\ln|x|-i\pi)^m}{1-x}dx\right]=0 \qquad (15)$$

from which we have

$$\Omega_m(t)\equiv\frac{1}{2\pi i}\int_{\alpha-i\infty}^{\alpha+i\infty}\frac{e^{st}\ln^m s}{1-s}ds$$
$$=\frac{1}{2\pi i}\int_0^\infty\frac{e^{-xt}(\ln x-i\pi)^m-(\ln x+i\pi)^m}{1+x}dx\ , \qquad (16)$$

where the change of variable $x\to -x$ has been performed in both the integrals of the right-hand side of Eq. (15).

It is easy to see that the quantity (16) can be written as

$$\Omega_m(t)=\int_0^\infty e^{-xt}\frac{1}{1+x}\times\sum_h^m(-1)^{(h+1)/2}\pi^{h-1}\binom{m}{h}(\ln x)^{m-h}dx\ , \qquad (17)$$

where $h=1, 3, 5, \ldots$ (odd integer). Since [see Eq. (9)]

$$\Omega_m(t)=\int_0^\infty e^{-tx}\omega_m(x)dx\ , \qquad (18)$$

where $\omega_m(x)$ is supposed to be a continuous function, the comparison of Eqs. (18) and (17) gives

$$\omega_m(x)=\frac{1}{1+x}\sum_h^m(-1)^{(h+1)/2}\pi^{h-1}\binom{m}{h}(\ln x)^{m-h}\ . \qquad (19)$$

Coming back to Eq. (12) and taking account of Eqs. (6), (9), (10), and the additivity property of the Laplace transform, we can write

$$\Omega(t)=\frac{1}{2\pi i}\int_{\alpha-i\infty}^{\alpha+i\infty}e^{st}\left(\frac{a}{e}\sum_{m=1}^{n}A_m\frac{\ln^m s}{1-s}\right)ds$$
$$=\frac{a}{e}\sum_{m=1}^{n}A_m\Omega_m(t)\ , \qquad (20)$$

where $\Omega_m(t)$ is given by Eq. (17).

Comparing Eq. (20) with Eq. (9), we find

$$\omega(x)=\frac{a}{e}\sum_{m=1}^{n}A_m\omega_m(x)\ , \qquad (21)$$

where $\omega_m(x)$ is furnished by Eq. (19).

Finally, inserting Eq. (21) in Eq. (5) we get the formula

$$N(kT\ln x)=\frac{ax+1}{ekT}\sum_{m=1}^{n}A_m\omega_m(x) \qquad (22)$$

for the density of states N.

In conclusion, the problem of the determination of the

density-of-states distribution in the gap of amorphous semiconductors is reduced to the determination of the analytical dependence of the induced charge density ρ on the band-bending potential $V(x)$; this can be done, for example, either by measuring the density charge at the insulator-semiconductor interface, $\rho(V_0)$, by capacitive techniques or by calculating $\rho(V_0)$ by field-effect measurements,[4] V_0 being the potential at the interface $(x=0)$. $\rho(V)$ can be obtained by fitting $\rho(V_0)$ data for different field voltage V_F, since[7]

$$V(x,V_0+\Delta V_0)=V(x-\Delta x,V_0) \quad .$$

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