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New Method of Determination of Density of States in the Pseudogap of Amorphous Semiconductor

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〈**Abstract**〉

Simple and direct method of calculation of the density of states in the pseudogap of amorphous semiconductor from the field-effect-conductance-change measurement is derived. There is no assumptions but finite temperature approximation. This theory is checked by such simplified assumptions as constant, parabolic and exponential density of states distributions and these prove that the theory is valid.

비정질 반도체의 상태 밀도를 결정하는 새로운 방법

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〈요　약〉

장효과 실험을 이용한 비정질 반도체의 에너지갭안에서의 상태밀도를 정하는 새롭고 간단한 방법을 구했다. finite-temperature 근사를 제외하고는 아무런 가정도 사용되지 않았다. 이 방법은 세개의 간단히 가정된 상태밀도 분포들—일정한 상태밀도, 포물형 상태밀도 그리고 지수형 상태밀도—에 의해 검토되었다. 이러한 검토 결과 이 이론은 타당하다는 것이 입증되었다.

Ⅰ. Introduction

The field effect experiment has been used to determine the gap-states-density of amorphous semiconductor. Spear et. al.[1] had firstly reported the density of states $N(E)$, from the fiel-effect-conductance-change data using the following three assumptions; a) parabolic or exponential band bending potential profiles, b) constant space charge density in a certain extent (abrupt approximation) and c) zero-temperature approximation. To remove any one of the above three assumptions, the iterative self-consistent method must be used. Chicago group[2]) had solved the Poisson's equation directly to find the band bending profile and integrated the space charge density to get the electric field in the sample and finally calculated currents with guessed $N(E)$. This calaulated current was compared with the experimental curent and $N(E)$ was fritted point by point, so they obtain a satisfied result. And others[3),4),5)] also developed the improved computer programs and found $N(E)$.

But all the methods above are ***indirect*** way of calaulating $N(E)$. In this paper we describe a new simple method to find $N(E)$ ***directly***

from the field-effect-conductance-change data of amorphous semiconductors. And the theory will be checked using three simplified assumptions i.e. constant, parabolic and exponential $N(E)$.

II. Theory of Analysis

The observed change in conductance is due to space charge layer caused by the applied gate voltage. If the gate voltage V_g is applied, the bands are bending. The band dending profiles can be given by Poisson's equation

$$\frac{d^2V(x)}{dx^2}=-\frac{\rho(x)}{\varepsilon_s} \qquad (1)$$

where ε_s is the electric permittivity of amorphous semiconductor and $\rho(x)$ is the space charge density at the distance x from the interface between insulator and amorphous semiconductor. We have for the space charge density

$$\rho(x)=(-e)\int_{-\infty}^{\infty}N(E)[f(E-eV(x))-f(E)]dE \qquad (2)$$

where $N(E)$ is the density-of-states distribution which is a function of energy E and $f(E)$ is the Fermi-Dirac distritribution function.

If the both sides of eq. (1) are multiplied by 2 $dV(x)/dx$ and integrated with respect to x, then

$$[F(V)]^2=\left[-\frac{dV(x)}{dx}\right]^2=-\frac{2}{\varepsilon_s}\int_0^V\rho(V')dV' \qquad (3)$$

wher $F(V)=-dV(x)/dx$, is the electric field of the amorphous semiconductor due to applied gate voltage V_g. And the specimen current I is given by

$$\frac{I-I_0}{I_0}=\frac{1}{d_s}\int_0^{d_s}\left[\exp\frac{eV(x)}{kT}-1\right]dx=\frac{1}{d_s}\int_0^{V_s}\frac{\left[\exp\frac{eV(x)}{kT}-1\right]}{F(V)}dV \qquad (4)$$

where I_0 is the current for the flat band condition, $V_s=V(x)|_{x=0}$ i.e. surface potential when the gate voltage V_g is applied, d_s is the thickness of amorphous semiconductor, e is the electronic charge, k is the Boltzmann constant and T is the themperature.

With eqs. (2), (3) and (4), we can obtain the localized states density in the pseudogap of amorphous semiconductor by computer interative self-consistent method with firstly guessed $N(E)$ and the $N(E)$ is fitted to match the calculated and experimental currents. But this method takes too much time and first of all, this is ***indirect*** way of calculating $N(E)$. Now we modify the all the equations above slightly and derive the ***simple*** and ***direct*** method of calculating the $N(E)$.

Since we can think that the specimen current I is a function of gate voltage V_g and the surface potential V_s is also a function of V_g, we can differentiate the both sides of eq. (4) with respect to gate voltage V_g, then

$$\frac{d_s}{I_0}\frac{\partial I}{\partial V_g}=\frac{\exp\left(\frac{eV_s}{kT}\right)-1}{F(V_s)}\frac{\partial V_s}{\partial V_g} \qquad (5)$$

where $F(V_s)=-dV(x)/dx|_{x=0}$.

Since $F(V_s)=(\varepsilon_{ox}/d_{ox}\varepsilon_s)(V_g-V_{FB})$ (6)

where ε_{ox} and d_{ox} are the electric permittivity and the thickness of insulator respectively and V_{FB} is the gate voltage for the flat band condition, then eq. (5) is modified by

$$\frac{d_s}{d_{ox}}\frac{\varepsilon_{ox}}{\varepsilon_s}\frac{V_g-V_{FB}}{I_0}\frac{\partial I}{\partial V_g}=\left[\exp\left(\frac{eV_s}{kT}\right)-1\right]\frac{\partial V_s}{\partial V_g} \qquad (7)$$

If we integrate the both sides of eq. (7) with respect to gate voltage V_g, then

$$(d_s\varepsilon_{ox})/(d_{ox}\varepsilon_s)\left[(V_g-V_{FB})\,I-\int_{V_{FB}}^{V_g}IdV_g\right]/I_0=\frac{kT}{e}\exp\frac{eV_s}{kT}-V_s-\frac{kT}{e} \qquad (8)$$

We can compute the left hand side numerically with the data of specimen current I vs. gate voltage V_g, and surface potential V_s will be determined. From eq. (6), we can show that

$$\frac{\partial^2[F(V_s)]^2}{\partial V_s^2} = 2\left(\frac{\varepsilon_{ox}}{d_{ox}\varepsilon_s}\right)^2 \quad (9)$$

Furthermore using finite temperature approximation, $\rho(V)$ is given by

$$\rho(V)=(-e)\left[\int_{E_f}^{E_f+eV} N(E)dE + \frac{\pi^2}{6}(kT)^2 \frac{dN(E)}{dE}\bigg|_{E_f}^{E_f+eV} + 0(kT)^4\right] \quad (10)$$

where E_f is Fermi energy.

From eqs. (3) and (10)

$$\frac{\partial^2[F(V_s)]^2}{\partial V_s^2} = -\frac{2}{\varepsilon_s}\frac{\partial\rho(V_s)}{\partial V_s} = \frac{2e^2}{\varepsilon_s}\left[N(eV_s) + \frac{\pi^2}{6}\left(\frac{kT}{e}\right)^2 \frac{\partial^2 N(eV_s)}{\partial V_s^2}\right] \quad (11)$$

In the last step, we set $E_f=0$. Since

$$\frac{\partial^2 F(V_s)}{\partial V_s^2} = 2\left(\frac{\varepsilon_{ox}}{d_{ox}\varepsilon_s}/\frac{\partial V_s}{\partial V_g}\right)^2 \quad (12)$$

then lefthand side of eq. (11) is calculated numerically using eqs. (8) and (12). If we solve the inhomogeous second order differential equation (11), we can calculate the density of states in the pseudogap of amorphous semiconductor ***directly*** from the field-effect-conductance-change data.

Ⅲ. Checks of the Theory Using Simple Assumptions

Checks of the theory proceed as follows;

1) from guessed $N(E)$, find the space charge density $\rho(V)$

2) differentiate $\rho(V_s)$ with respect to V_s

and 3) compare with direct calculation of eq. (11)

1. Constant Density of States

If the density of states is constant i.e. $N(E)=N_0$, by eq. (10), space charge density is given by

$$\rho(V_s) = -N_0 e^2 V_s \quad (13)$$

therefore

$$\frac{\partial^2[F(V_s)]^2}{\partial V_s} = -\frac{2}{\varepsilon_s}\frac{\partial\rho(V_s)}{\partial V_s} = \frac{2e^2}{\varepsilon_s}N_0 \quad (14)$$

And from eq. (11)

$$\frac{\partial^2[F(V_s)]^2}{\partial V_s^2} = \frac{2e^2}{\varepsilon_s}N_0 \quad (15)$$

Eqs. (14) and (15) are corresponding exactly with each other.

2. Parabolic Density of States

We assume that $N(E)=N_0[(E-E_f)/kT]^2$, then the space charge density is given by

$$\rho(V_s) = -[N_0(eV_s)^3(kT)^2 + \pi^2 N_0 eV_s/3] \quad (16)$$

therefore

$$\partial^2[F(V_s)]^2/\partial V_s^2 = (2e^2/\varepsilon_s)N_0[(eV_s/kT)^2+\pi^2/3] \quad (17)$$

And from eq. (11)

$$\partial^2[F(V_s)]^2/\partial V_s^2 = (2e^2/\varepsilon_s)N_0[(eV_s/kT)^2+\pi^2/3] \quad (18)$$

Eqs. (17) and (18) are corresponding exactly with each other

3. Exponential Density of States

And now we assume that $N(E)=N_0 \exp\{(E-E_f)/kT\}$, then the space charge density is given by

$$\rho(V_s) = -eN_0 kT(1+\pi^2/6)\{\exp(eV_s/kT)-1\} \quad (19)$$

thus

$$\partial^2 F(V_s)^2/\partial V_s^2 = (2e^2/\varepsilon_s)\, N_0 \exp(eV_s/kT)\cdot(1+\pi^2/6) \quad (20)$$

From eq. (11)

$$\partial^2 F(V_s)^2/\partial V_s^2 = (2e^2/\varepsilon_s)\, N_0 \exp(eV_s/kT)\cdot(1+\pi^2/6) \quad (21)$$

Eqs. (20) and (21) are corresponding exactly with each other.

Ⅳ. Conclusions

The direct method of calculation of density of states $N(E)$, in the pseudogap of amorphous semiconductor is described. From this method,

we can evaluate the $N(E)$ using the field-effect-conductance-change measurement without any assumptions but finite-temperature approximation for finding the space charge density. Integrating the specimen current with respect to gate voltage, we can find the relation between surface potential and gate voltage. This relation is differentiated doubly to get a constant value of the second order inhomogeneous differential equation which is used in calculation of $N(E)$.

Three simplified assumptions for density of states (constant, parabolic and exponential density of states distributions) are used to check the theory. It is proved that the theory is valid.

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