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Model calculation on the Meyer-Neldel rule for the field-effect conductance of hydrogenated amorphous silicon

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A model calculation was carried out to study the Meyer-Neldel rule of the field-effect conductance of hydrogenated amorphous silicon (a-Si:H). It was found that the shift of Fermi level and the potential profile in the sample with temperature can explain the Meyer-Neldel rule if a model density of states of a-Si:H is properly chosen. So it is of doubt to think that the conductivity prefactor varies in a single sample of band-bending case, as assumed by some authors.

It is well known that the pre-exponential factor of dark conductivity of hydrogenated amorphous silicon (a-Si:H) obeys the Meyer-Neldel rule (MNR), which states that

\[ \sigma_0 = \sigma_{00} \exp(\alpha d), \]

where \( \sigma_0 \) and \( E_g \) are the experimentally determined conductivity prefactor and activation energy, respectively, and \( \alpha \) is typically between 14 and 31 eV \(^{-1}\). The MNR holds whenever the activation is altered by such methods as doping, light soaking, and field effect. The origin of the MNR is not yet clear and has been attributed to such mechanisms as the shift of mobility edge, surface band bending, electron-phonon interaction, and statistical shift of the Fermi level.

Another related problem is whether the conductivity prefactor varies in a single sample when the activation energy is a function of position, or the MNR is not a local property but is apparently satisfied for the sample as a whole in the case of band bending. To study this problem, we assume that the conductivity prefactor is of a single value in a sample and work out a model calculation on the temperature dependence of the a-Si:H field-effect conductance.

The model sample in this work is a thin film throughout which the model density of states (DOS) in Fig. 1 is valid. The electric potential varies along the x direction as shown in the insert of Fig. 1. The effects of external field and of surface states are represented by the boundary conditions of the potential at \( x = 0 \). A single conductivity prefactor for \( 0 \leq x < d \), where \( d \) is sample thickness, \( d = 5000 \) Å. The boundary condition at \( x = d \) in field-effect analysis is

\[ V = 0 \quad \text{and} \quad \frac{dV}{dx} = 0 \quad \text{as} \quad x \rightarrow d. \]

The amount of band bending at \( x \) is determined by the Poisson's equation

\[ \frac{d^2V}{dx^2} = \frac{\epsilon}{\epsilon_0} \int_0^{N(E)} \left[ f[E - V(x)] - f(E) \right] dE, \]

where \( \epsilon \) is the permittivity of a-Si:H, \( N(E) \) is the DOS, \( f \) is the Fermi distribution function, and \( V(x) \) is measured in eV. If a DOS is given, we can obtain \( V(x) \) satisfying conditions (2), by solving Eq. (3) numerically. In doing this it is useful to note that the asymptotic behaviors of \( V \) and \( dV/dx \) are related to each other as \( x \rightarrow d \) or \( V \rightarrow 0 \): as \( V \rightarrow 0 \), Eq. (3) becomes approximately

\[ \frac{d^2V}{dx^2} = \frac{\epsilon}{\epsilon_0} N^0(E) V, \]

where \( N^0(E) \) would be the “zero temperature equivalent” DOS of \( N(E) \) if we used the zero temperature statistics on the right-hand side of Eq. (3) and can be obtained by

\[ N^0(E_F + V) = \int_{-\infty}^{E_F} dE N(E) \left[ \frac{\partial f(E - V)}{\partial V} \right]. \]

Equation (4) is easily solved as \( x \rightarrow d \):

\[ V(x) \propto \exp(-Kx), \quad \frac{dV}{dx} = -KV, \]

where \( K = [\epsilon N^0(E_F)/\epsilon_0]^{-1/2} \). Thus, it is easier to integrate Eq. (3) starting at \( x = d \), since then we need only one boundary value, say \( V(d) \).

When the temperature rises, the Fermi distribution

\[ \text{FIG. 1. Model density of states of a-Si:H used in this work. Enclosed in the box is the conduction-band diagram in real space of our model sample, where } V(x) \text{ is the electric potential measured in energy unit. The numerical values of density of states are (in eV \(^{-1}\) cm \(^{-3}\) and energy in eV): } 10^9 \text{ for } E \leq -1.6 \text{ and } E > -0.15 \text{, } 10^7 \exp[10(E + 0.15)] \text{ for } -0.45 \leq E < -0.15 \text{, } 10^6 \exp[45.4(0.65 + E)] \text{ for } -0.8 \leq E < -0.45 \text{, } 10^4 \exp[17.9(E + 1.0)] \text{ for } -1.0 \leq E < 0.8 \text{, } 10^2 \text{ for } -1.2 < E < -1.0 \text{, and } 10^2 \exp[23.0(E + 1.6)] \text{ for } -1.6 < E < -1.2. \]

\[ \text{(2)} \]

\[ \text{(3)} \]

\[ \text{(4)} \]

\[ \text{(5)} \]
functions $f$ and $E_F$ change, and so does the potential profile. But the total number of electrons is conserved, and we may write

$$\int dx \, dE \, N[E + V(x)] \, f(E, E_F, \tau) = \text{constant},$$  \hspace{2cm} (7)

$$\frac{dE_F}{d\tau} = - \int dx \, dE \, \left[ \frac{N(E + V) f(1 - f)(E - E_F)}{\tau} + \frac{dN(E + V)}{dE} \frac{f(E, E_F)}{\tau} \right] \left[ \int dx \, dE \left[ N(E + V) f(1 - f) + \frac{dN(E + V)}{dE} \frac{f(E, E_F)}{\tau} \right] \right].$$  \hspace{2cm} (8)

With a given DOS we may proceed using Eq. (8) to calculate the temperature dependence of the conductance of the model sample as follows.

(i) Obtain $V(x)$ at initial $\tau$.

(ii) Find $\frac{\partial V}{\partial \tau}$ and $\frac{\partial V}{\partial E_F}$ from the calculations of the potential variations with small variations of $\tau$ and $E_F$, respectively. In this step the following boundary condition should be used, which represents the constancy of the gate voltage in the field-effect geometry:

$$\frac{dV}{dx} = \text{constant} \quad \text{at} \quad x = 0 \quad \text{as} \quad \tau \quad \text{and/or} \quad E_F \quad \text{varies}.$$  \hspace{2cm} (9)

(iii) Calculate $\frac{dE_F}{d\tau}$ and obtain $E_F$ at a slightly higher temperature. At this higher $\tau$, calculate $V(x)$ using condition (9). Now go to step (ii) to continue.

The conductance is calculated at each temperature by

$$G = \text{constant} \int_0^\tau dx \, \exp \left( - \frac{[E_c - V(x) - E_F]}{\tau} \right).$$  \hspace{2cm} (10)

In Fig. 2 the field-effect conductance of our model sample is calculated, assuming $E_F = -0.85$ eV at $\tau = 0.026$ eV, and plotted against $1/T$, and in Fig. 3 the apparent conductance prefactor, against activation energy. The conductance curves are nearly straight lines and the MNR is satisfied with

$$A = 23 \text{ eV}^{-1} \text{ for } 0.25 < E_a < 0.6 \text{ eV}.$$  

The results can be interpreted as follows. The conductance may be written empirically, letting $E_c = 0$,

$$G = G_0 \exp \left( \frac{\bar{V} + E_F}{\tau} \right),$$  \hspace{2cm} (11)

where $\bar{V}$ is the effective decrease of activation energy due to band bending and is temperature dependent. The apparent pre-exponential factor becomes in this case

$$G_0 = G_{00} \exp \left( \frac{dV}{d\tau} + \frac{dE_F}{d\tau} \right).$$  \hspace{2cm} (12)

To estimate $d\bar{V}/d\tau$, it is fairly satisfactory to consider the shift of $V(0)$ with temperature. In Fig. 4, $V(0)$ is plotted against $\tau$ for the conductances in Fig. 2, and also written are $\Delta V(0)/\Delta \tau$ and $\Delta E_F/\Delta \tau$, the mean shifts of $V(0)$ and $E_F$ for $\tau$ between 0.026 and 0.03 eV. As the activation energy becomes smaller (or $\bar{V}$ larger), $E_F$ increases at a higher rate with temperature, but this causes $\bar{V}$ to decrease still more rapidly, which results in smaller $d\bar{V}/d\tau + dE_F/d\tau$.

In summary, we have shown by a numerical method that the MNR of the field-effect conductance of $a$-Si:H can be explained by the temperature shift of $E_F$ and the potential profile. This, together with our previous work, tells us that the statistical shift of $E_F$ is at least one of the major reasons for the empirical MNR of $a$-Si:H. Furthermore, it is unnec-
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