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THE QUANTUM AND THE CLASSICAL CALCULATIONS OF D/μ RATIO IN THE MOSFET STRUCTURE IN THE PRESENCE OF THE IMAGE EFFECT

In order to determine the ratio of diffusion constant D and mobility μ (the Einstein relation) it is necessary to solve self-consistently the Shrödinger and Poisson equation. In some cases, it is sufficient, in order to determine ratio D/μ, to analyse the problem in the clasical way solving only the Poisson equation. The paper contains the comparison of results, obtained in both ways, depending on the MOSFET structure parameters and on temperature.

Due to different dielectric constants of the semiconductors and the oxide the image effect affects the D/μ ratio.

1. INTRODUCTION. The initial step in the study of properties (transport, optical,..) of the carriers in the inversion layer is the determination of the potential distribution along the layer. For an accurate determination of this distribution the self-consistent method for solving the Schrödinger and Poisson equation is used [1]. This method takes into account all quantum-mechanical properties of the carriers. The potential distribution may be determined by solving the Poisson equation in the classical form [2]: the so obtained solution has , more or less, an approximative character [3,4].

The present paper analyses the Einstein relation (the ratio of diffusion constant D and mobility μ) derived by both the quantum-mechanical and the classical procedure. The comparison of numerical results may provide useful information on the applicability of the classical procedure.

A particular attention will be devoted to the influence image effect on the Einstein relation. It will be shown to which extent this effect is dominant.

2. THEORY AND THE NUMERICAL RESULTS. Let us assume the z-axis to be normal to the surface of the semiconductor-dielectric and the plane z=0 represents the surface. Electrostatic potential $\phi(z)$ represents the solution of the Poisson equation,

under the respective boundary conditions:

$$\frac{d^2\phi(z)}{dz^2} = \frac{e}{\varepsilon_s}(N_A+n(z)), \quad \phi(0)=0 \text{ and } \left.\frac{d\phi}{dz}\right|_{z=0} = -\frac{e}{\varepsilon_s}(N_{inv}+N_A W) \quad (1.$$

where e is the electron charge, ε_s the dielectric constant of the semiconductor, N_A the acceptors concentration, N_{inv} the surface density of electrons, n(z) electron concentration and W the width of the space charge region.

In order to find $\phi(z)$ from (1), it is necessary to know the form of dependence n(z). In the classical case it is[2]:

$$n(z) = 2\cdot n_v\left(\frac{m_d kT}{2\pi\hbar^2}\right)^{3/2} F_{1/2}\left(\frac{E_F-e\phi(z)}{kT}\right) \quad (2)$$

where m_d is the density of states effective mass of the conduction band, n_v is the equivalent conduction valley degeneracy factor, E_F is the Fermi energy, while k,T and $\hbar$ have their usual meaning. $F_{1/2}$ is the conventional Fermi-Dirac integral.

In the case of the quantum-mechanical treatment n(z) is [2]:

$$n(z) = \sum_{i,j} \frac{m_{dj}\, kT}{\pi\hbar^2} \ln\left(1+\exp\left(\frac{E_F-E_i^j}{kT}\right)\right)\cdot|\psi_i^j(z)|^2 \quad (3)$$

where m_{dj}, E_i and $\psi_i^j(z)$ are density of states effective mass, energy and electron wave function at the i-th energy level in the vicinity of the j-th energy minimum. The appearance of $\psi_i^j(z)$ and E_i^j in expression (3) requires the solving of Schrödinger equation, which, on its part, leads to an indispensable self-consistent solving of Poisson and Schrödinger equation.

A two-dimensional electron gas is formed in the inversion layer. Starting from the Boltzmann kinetic equation it could be shown that the ratio of diffusion constant D and mobility μ of this 2D electronic gas is given by expression [5]:

$$D/\mu = \frac{1}{e}\frac{N_{inv}}{\partial N_{inv}/\partial W_F}, \quad N_{inv} = \int_0^{+\infty} n(z)dz \quad (4)$$

where W_F is the chemical potential.

Expression (4) in the case of the classical treatment passes into

$$D/\mu = \frac{kT}{e}\frac{\int_0^{+\infty} F_{1/2}(\eta)dz}{\int_0^{+\infty} F_{-1/2}(\eta)dz}, \quad \eta \equiv \frac{E_F-e\phi(z)}{kT} \quad (5)$$

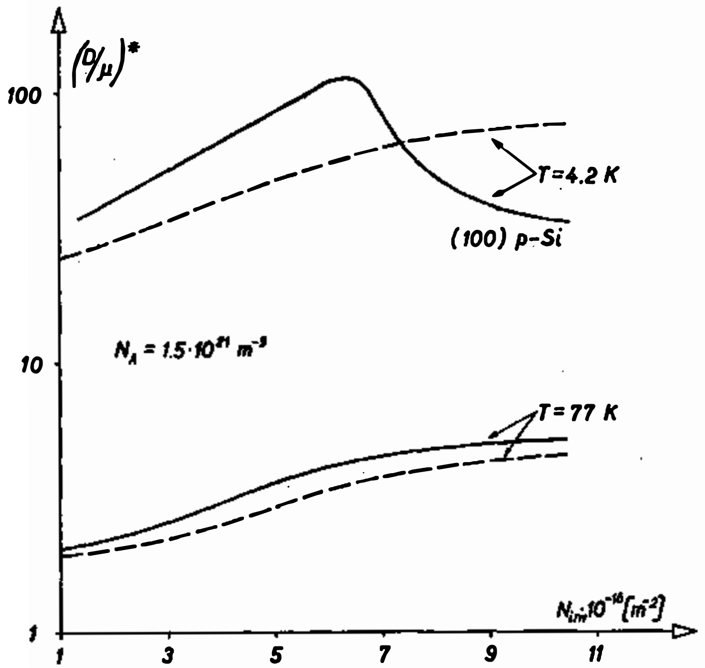

Fig.1. - The ratio $(D/\mu)^* = D/\mu/kT/e$ as function of N_{inv} at T = 4.2K and t = 77K (the full line represents the results obtained by a self-consistent solving; the dotted line - those obtained by a classical method).

The case of the quantum solution in "gradual-channel appxoximation" gives to expression (4) the form [5]:

$$D/\mu = \frac{\hbar^2 N_{inv}}{e} \left[\left| \sum_{i,j} m_{dj} \; 1+\exp \frac{E_i^j - E_F}{kT} \right| ^{-1} \right]^{-1} \qquad (6)$$

where D and μ are the effective values of these quantities [5]:

$$\mu = \sum_{i,j} \mu_i N_i^j / N_{inv}; \quad D = \frac{\sum_{i,j} D_i \frac{dN_i^j}{dW_F}}{\frac{\partial N_{inv}}{\partial W_F}} \qquad (7)$$

Due to the existence of different dielectrical constants of dielectric ε_{ox} and semiconductors ε_s, the image efects must be taken into account. The additional potential energy, due to this effect is given by expression [6]:

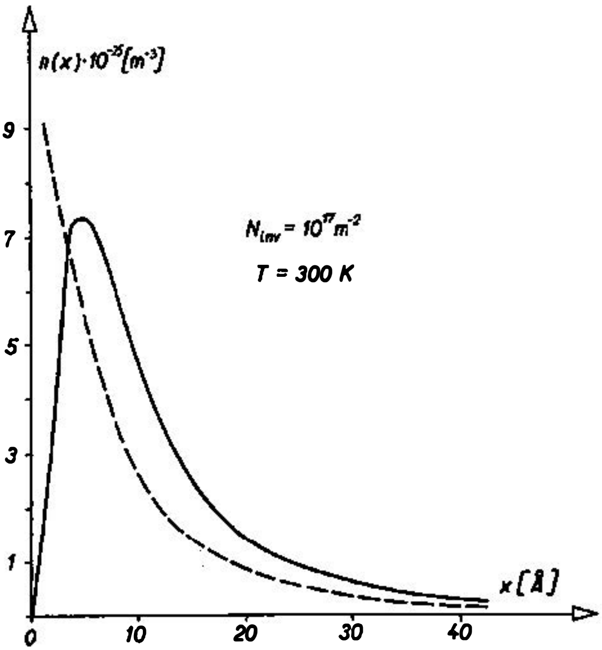

Fig.2. - Dependence of concentration n(x) at $N_{inv}=10^{17}m^{-2}$ and T=300K (the full - the classical solution in the presence of the image effect, the dotted line - the classical solution).

$$U_{img}(z) = = -e\phi_{img}(z) = \frac{\varepsilon_s-\varepsilon_{ox}}{\varepsilon_s+\varepsilon_{ox}} \frac{e}{16\pi\varepsilon_s z} . \qquad (8)$$

The numerical calculations were performed for (100)Si inverse layer of the uniform concentration of acceptors $N_A=1.5\cdot10^{21}m^{-3}$ in the large temperature range and surface densities. Energies E_i are determined by a QR transformation method, while potencial$\phi(z)$ from (1) and (2) is determined by the Runge-Kutta method. Fig.1 displays the dependence of ratio $(D/\mu)^* \frac{D/\mu}{kT/e}$ on N_{inv} for the case of quantum and classical treatment and for temperatures T=4.2K and T=77K. The cases of higher temperatures are not of particular interest, because then $(D/\mu)^*\to1$, and the difference becomes negligible. Fig.2 displays the dependences of concentration n(z)by classical treatment. The numerical calculations show that the influence of the image effect on $(D/\mu)^*$ is negligible and therefore is not presented in figures: for example $(D/\mu)^*$ at $N_{inv}=10^{17}m^{-2}$ and T=77K, determined self-consistently yields to 4.56, without the image effect while it is 4.51 in the presence of the effect.

Our numerical calculations show that the image effect changes does not exceed 5%.

4. CONCLUSION

This paper makes a comparative analysis of the Einstein relation in the inversion layer for the cases of the classical and the quantum treatments of the problem.

The numerical results (Fig.1) show that the classical treatment is applicable to the determination of the Einstein relation for higher temperatures and smaller surface concentrations. At lower temperatures (especially at T=4.2K the dependence $(D/\mu)^*$ obtained in the classical way does not follow qualitatively the respective dependence obtained self-consistently. The following inference follows: The ratio D/μ determined in a classical way qualitatively and quantititatively agrees with D/μ determined in a quantum manner, if the quantization conditions were less prononced.

The influence of the image effect to the Einstein relation is almost negligible (<5%). However, the influence on the concentration distribution and potential is considerable. Fig.2 shows that the concentration distribution in the presence of the image effect (determined in the classical way) has a qualitative shape as if it were determined in the quantum treatment. The pronounced maximum at 5Å from the surface in clearly visible.

REFERENCES

[1] G.Dorda: Festkörperprobleme XIII,215 (1873)

[2] F.Stern: Proc., 10th Int.Conf.Phys.Sem.451, Cambridge, Massachusetts (1970)

[3] Y.Weissman: J.Phys. C 9, 2353 (1976)

[4] Y.Weissman: Phys.Lett. 59A, 343 (1976)

[5] D.Tjapkin, V.Milanović, Ž.Spasojević (to be publis hed)

[6] F.Ohkawa, Y.Uemura; Progr.Theor.Phys.Suppl, 57, 164(1975)