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COMMENT ON "FIELD PENETRATION AND BAND BENDING NEAR SEMICONDUCTOR SURFACES IN HIGH ELECTRIC FIELD" BY T.T. TSONG

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Abstract - It is well known that the surface of specimen in field ion microscope is applied high electric field and that field penetration and band bending must be considered for proper interpretation of atom probe data of semiconductors as investigated by some researchers. Above all, because of surface temperature rise by laser irradiation, it is necessary to gain knowledge about the relation between field penetration and temperature of semiconductor surface. The problem has already been tried to be solved and the results of numerical calculation under various conditions were reported many years ago. However, in the paper, besides the wrong result with regard to field penetration, significant errors seem to exist in the procedures of numerical calculations. This can be easily confirmed by comparison with analytical solutions in case of intrinsic semiconductor under the conditions similar to that in the paper.

Recently atom probe using a laser unit, one of the applications of field ion microscope, has been indispensable to the investigation of semiconductor surfaces /1/. It is well known that the surface of specimen in field ion microscopy is applied high electric field and that field penetration and band bending must be considered for proper interpretation of atom probe data of semiconductors as investigated by some researchers /2-5/. Above all, because of surface temperature rise by laser irradiation, it is necessary to gain knowledge about the relation between field penetration and temperature of semiconductor surface. The problem has already been tried to be solved and the results of numerical calculations under various conditions were reported many years ago /2/. However, in the paper /2/, significant errors seem to exist in the procedures of numerical calculations. This can be confirmed easily by comparison with analytical solutions in case of intrinsic semiconductor under the conditions similar to that in the paper /6/.

In order to determine the exact value for the band bending as expressed the potential $V(z)$, we have only to solve Poisson's equation (1) assuming that the semiconductor-vacuum interface is considered to be infinitive x-y plane.

$$\frac{d^2 V(z)}{dz^2} = \frac{\rho}{\varepsilon_r \varepsilon_0},$$

(1)

where $\rho$ is the charge distribution, $\varepsilon_r$ is the dielectric constant of semiconductor, $\varepsilon_0$ is the permittivity of the vacuum and the potential $V(z)$ is defined by equation

$$qV(z) = E_f - E_i,$$

(2)
where \( q \) is the magnitude of the electron charge, \( E_f \) is Fermi level and \( E_i \) is parallel to the band edges and in the bulk coincides with the intrinsic level. If we assume that the carrier densities are governed by the Maxwell Boltzmann distribution,

\[
\rho = -2qn_i \sinh\left(\frac{qV(z)}{kT}\right),
\]

where \( k \) is the Boltzmann constant, \( T \) is the temperature of the semiconductor and \( n_i \) is the intrinsic carrier density given to be

\[
n_i = (n_e n_v \exp\left(-\frac{E_g}{kT}\right))^\frac{1}{2},
\]

where \( n_e \) is the effective density of states in conduction band, \( n_v \) is the effective density of states in valence band and \( E_g \) is the energy gap of the semiconductor. This assumption holds if the potential is less than about 0.5 volts. Therefore, the surface electric field is here chosen to satisfy this condition. Without this assumption, we cannot obtain the analytical solution showing the relation between surface potential and temperature. However, this limits the model described here to fields below those which apply in the case of field ionization or even field electron emission.

With the help of eq. (3), Poisson's equation (1) can be integrated once \( /7/ \) and be solved analytically to give

\[
V(z) = \frac{4kT}{q} \arctanh\left(\exp\left(-\frac{z}{L_D}\right) \tanh\left(\frac{qV_s}{4kT}\right)\right),
\]

where \( L_D \) is known as Debye length given to be

\[
L_D = \left(\frac{\varepsilon \varepsilon_0 kT}{2q n_i}\right)^\frac{1}{2},
\]

and \( V_s \) is surface potential given to be

\[
V_s = \frac{2kT}{q} \arcsinh\left(-\frac{E_s}{8n_i kT}\right),
\]

where \( E_s \) is the surface electric field.

In a similar way, the field penetration can be expressed as electric field \( E(z) \) within the surface charge region to be calculated from

\[
E(z) = -\frac{2kT}{qL_D} \sinh\left(2\arctanh\left(\exp\left(-\frac{z}{L_D}\right) \tanh\left(\frac{1}{2} \arcsinh\left(-\frac{E_s}{8n_i kT}\right)\right)\right)\right).
\]

The above solutions give estimation of an interest. As shown in fig. 1, the surface potential decreases with temperature. This is clearly opposed to the numerical calculation in the paper \( /2/ \). It is out of question that different parameters give quantitative difference: the very problem is that the qualitative relation between surface potential and temperature estimated by Tsong is different from that of the above analytical
Fig. 1. Surface potential of intrinsic silicon at $z = 0$ as a function of the temperature. Solid curve: $E_s = 1 \times 10^4$ V/cm. Dashed curve: Tsong's result ($E_s = 10^7$ V/cm) /2/.

Fig. 2. Field strength in intrinsic silicon at $z = 5\text{Å}$ as a function of the temperature. Solid curve: $E_s = 1 \times 10^4$ V/cm. Dashed curve: Tsong's result ($E_s = 10^7$ V/cm) /2/. 
solutions. Thus, significant errors seem to exist in the procedures of numerical calculations. On the other hand, eq. (8) indicates that the field strength near surface is deeper at higher temperature as shown in fig. 2, which agrees well to the paper /2/ regardless of the quantitative difference. However, the field strength at deeper depth decreases with temperature as shown in fig. 3.

As mentioned above, there are a few serious problem in the paper /2/, but not in case of Nernst's work taking account of surface states /5/. By the way, all parameters necessary for calculations are based on the data in the ref. /8/.

References