Charge-carrier mobility in hydrogen-terminated diamond field-effect transistors

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Diamond field-effect transistors (FETs) have potential applications in power electronics and high-output high-frequency amplifications. In such applications, high charge-carrier mobility is desirable for a reduced loss and high-speed operation. We have recently fabricated diamond FETs with a hexagonal-boron-nitride gate dielectric and observed a high mobility above 300 cm²V⁻¹s⁻¹. In this study, we examine which scattering mechanism limits the mobility of our FETs through theoretical calculations. Our calculations reveal that the dominant carrier scattering is caused by surface charged impurities with the density of ≈1×10¹² cm⁻², and suggest a possible increase in mobility over 1000 cm²V⁻¹s⁻¹ by reducing the impurities.
I. INTRODUCTION

Diamond has attracted much attention as a next-generation semiconducting material because of its excellent properties such as a wide-band gap, high thermal conductivity, high breakdown electric field, and high mobility. These properties enable field-effect transistors (FETs) to operate at high temperature with low-energy loss, to resist a high voltage, and to be reduced in size. Previously, an FET operation at 400°C and a high breakdown voltage above 2000 V were reported. Diamond FETs in previous studies were often fabricated using hydrogen-terminated diamond surface, which exhibits a p-type surface conductivity.

The p-type surface conductivity appears on hydrogen-terminated diamond after air exposure even if the diamond is non-doped. The surface conductivity can be explained by a transfer doping model. The valence band maximum of hydrogen-terminated diamond is higher than the lowest unoccupied states of impurities adsorbed on the diamond surface by air exposure. The electrons in the valence bands of diamond are therefore transferred to the impurities and holes are induced at the diamond surface, resulting in the surface conductivity. It is known that the transfer doping is also caused by the exposure to NO gas and the deposition of a solid insulator with a high electron affinity such as V$_2$O$_5$.

The mobility of the surface conductivity of hydrogen-terminated diamond is typically 10-100 cm$^2$V$^{-1}$s$^{-1}$ at room temperature. This value is more than one order of magnitude lower than the intrinsic mobility of bulk diamond ($\approx$4000 cm$^2$V$^{-1}$s$^{-1}$). Recently, Li et al. calculated the mobility of the surface conductivity of hydrogen-terminated diamond as a function of temperature and carrier density. They pointed out that the major scattering source was the surface impurity.

The mobilities of the hydrogen-terminated diamond FETs are almost the same as or less than that of the surface conductivity of hydrogen-terminated diamond. This suggests that the charged impurities also exist in the gate insulator. In fact, it was suggested that Al$_2$O$_3$ film deposited by the atomic layer deposition (ALD) method contains oxygen point defects and aluminum vacancies, and electrons trapped in these defects are balanced with hole carriers in diamond. Other gate insulators such as SiO$_2$ and CaF$_2$ were formed by vacuum evaporation or sputter deposition, but these films are amorphous and may also contain charged impurities and traps.

Recently, we fabricated diamond FETs using a monocrystalline hexagonal boron nitride
(h-BN) as a gate insulator and observed a high mobility above 300 cm²V⁻¹s⁻¹. The high mobility is presumably due to a low density of charged impurities in h-BN. In this study, we calculated the room-temperature mobility of diamond FETs as a function of carrier density to reveal the mobility limiting factor in our FETs.

II. MODELING

The equations we used for calculating the scattering rate were basically the same as those used in the paper by Li et al. There are, however, two major differences between our calculation and theirs. First, Li et al. assumed that the density of surface charged impurities was the same as the carrier density. This is reasonable for the surface conductivity of hydrogen-terminated diamond because negative charges of the surface impurities are balanced with the positive charges of holes in diamond according to the transfer doping model. In diamond FETs, however, the density of surface charged impurity is independent of the carrier density because the carrier density can be controlled by the gate voltage. We therefore treated the density of surface charged impurities as a constant. This treatment causes a qualitative difference between the carrier density dependence of mobility in our calculation and that in the paper of Li et al.

The second different point is the way to treat three valence bands. Li et al. used a single equivalent isotropic band model. That is, they assumed a single effective band with the density-of-state mass $m^*_d = ((m^{1H})^{3/2} + (m^{HH})^{3/2} + (m^{SO})^{3/2})^{2/3}$, and the conduction mass $m^*_c = ((m^{1H})^{3/2} + (m^{HH})^{3/2} + (m^{SO})^{3/2})/((m^{1H})^{1/2} + (m^{HH})^{1/2} + (m^{SO})^{1/2})$. (They used the heavy hole (HH) mass $m^{HH} = 0.588m_0$, the light hole (LH) mass $m^{1H} = 0.303m_0$, and the split-off (SO) hole mass $m^{SO} = 0.394m_0$, $m_0$ being the rest mass.) In contrast, we distinguished the three bands and performed the calculation of the mobilities for the three bands separately. The distribution of the carrier densities to the HH, LH, and SO bands was determined by solving Schrödinger and Poisson equations self-consistently:

$$\left[ -\frac{\hbar^2}{2m^*_i} \frac{d^2}{dz^2} + e\phi(z)(+\Delta^{SO}) - E^i_n \right] \Psi^i_n(z) = 0, \quad (1)$$

$$\frac{d^2\phi(z)}{dz^2} = -\frac{1}{\epsilon_0\epsilon_s} \left[ eN_{\text{depl}} + e \sum_{i,n} n^i_n \left| \Psi^i_n(z) \right|^2 \right], \quad (2)$$

$$n^i_n = \frac{m^i/k_B T}{\pi\hbar^2} \ln \left[ 1 + \exp \left( \frac{E_F - E^i_n}{k_B T} \right) \right], \quad (3)$$
Here, $e$ is the elementary charge, $\epsilon_0$ is the vacuum permittivity, $\epsilon_s$ is the static dielectric constant of diamond, $e\phi(z)$ is the potential energy, $N_{\text{depl}} = N_D - N_A$, $N_D$ and $N_A$ are the ionized donor and acceptor concentration in the diamond substrate, $E_n^i$ is the maximum energy of the $n$th sub-band, $\Psi_n^i(z)$ is the wave function corresponding to $E_n^i$, $n_n^i$ is the sheet hole density of the $n$th sub-band, $E_F$ is the Fermi level, $k_B$ is the Boltzmann constant, and $T$ is the absolute temperature. We did not consider the band mixing of the HH, LH, and SO subbands. The carrier density ($n_{\text{HH}}^i$, $n_{\text{LH}}^i$, and $n_{\text{SO}}^i$) for HH, LH, and SO holes were obtained by the summation of densities over the seven lowest subbands ($n_{\text{max}} = 7$). The summation of the 1st HH, LH, and SO subbands reaches >89% of the total carrier density ($n_{\text{tot}} = n_{\text{HH}} + n_{\text{LH}} + n_{\text{SO}}$) in the range of a total carrier density between $1 \times 10^{11}$ and $1 \times 10^{14}$ cm$^{-2}$ (Fig. 1(b)). $\Delta_{\text{SO}}$ is the spin-orbit gap energy and is taken into account only in the calculation for split-off holes. $\Delta_{\text{SO}}$ of diamond is 6 meV$^{11}$ A secondary ion mass spectrometry measurement on a diamond substrate similar to the ones we used for fabricating the FETs indicated that the concentration of nitrogen which works as a donor is 0.5 ppm and that of boron which works as an acceptor is 5 ppb. Although there may be some defects (e.g. vacancies) that influence the value of $N_{\text{depl}}$, we assumed $N_{\text{depl}} = 0.5$ ppm. We used the following values of effective masses obtained from Luttinger parameters$^{12}$ for the (111) diamond surface:

\begin{align*}
m_{z}^{\text{HH}} / m_0 &= 1/(\gamma_1 - 2\gamma_3) = 0.763, \\
m_{z}^{\text{LH}} / m_0 &= 1/(\gamma_1 + 2\gamma_3) = 0.248, \\
m_{z}^{\text{SO}} / m_0 &= 1/\gamma_1 = 0.375, \\
m_{//}^{\text{HH}} / m_0 &= 1/(\gamma_1 + \gamma_3) = 0.299, \\
m_{//}^{\text{LH}} / m_0 &= 1/(\gamma_1 - \gamma_3) = 0.503, \\
m_{//}^{\text{SO}} / m_0 &= 1/\gamma_1 = 0.375.
\end{align*}

$m_{z}^i$ is the effective mass along the $z$ direction perpendicular to the diamond surface, and $m_{//}^i$ is the effective mass parallel to the diamond surface.

We then calculated the scattering rate for the heavy-, light-, and split-off holes. We considered three scattering mechanisms for calculating the scattering rate: the surface impurity scattering, acoustic phonon scattering, and surface roughness scattering. The optical phonon
scattering was not considered because the optical phonon energy is as large as 165 meV and the occupation number of optical phonons is small at room temperature in diamond\textsuperscript{[13]}. The effect of background ionized impurities is small and also neglected. (The contribution of the background ionized impurities to mobility is more than one order of magnitude smaller than that of surface charged impurities for the carrier density larger than $1 \times 10^{12} \text{cm}^{-2}$.) We note that the donors and acceptors should be fully ionized near the surface because of the band bending.

The equations of the scattering rate for three different scattering mechanisms are described below.

1. Surface charged impurity scattering

The carriers are scattered by the Coulomb potential arising from charged impurities on the surface. The scattering rate caused by the surface charged impurities is given by

$$
\frac{1}{\tau_{\text{imp}}^{i}} = n_{\text{imp}} \frac{m_{i}^{\text{eff}}}{2\pi\hbar^{3}(k_{F}^{i})^{3}} \left( \frac{e^{2}}{2\epsilon_{0}\epsilon_{s}} \right)^{2} \int_{0}^{2k_{F}^{i}} \frac{\exp(-2qd)}{[q + q_{TF}^{i}G(b^{i}, q)]^{2} \left( \frac{b^{i}}{b^{i} + q} \right)^{6}} \frac{q^{2}dq}{\sqrt{1 - (q/2k_{F}^{i})^{2}}} \right). \quad (11)
$$

$n_{\text{imp}}$ is the density of surface charged impurity, $\hbar$ is the reduced Planck constant, $q_{TF}^{i} = m_{i}^{\text{eff}} e^{2}/(2\pi\epsilon_{0}\epsilon_{s} \hbar^{2})$ is the Thomas-Fermi screening wave vector, $G(b^{i}, q) = 1/8\{2[b^{i} / (b^{i} + q)]^{3} + 3[b^{i} / (b^{i} + q)] + 3[b^{i} / (b^{i} + q)]^{2} \}$ is a form factor, $b^{i} = [33\pi m_{i}^{\text{eff}} e^{2} n^{i} / (2\hbar^{2}\epsilon_{0}\epsilon_{s})]^{1/3}$ is a parameter in a Fang-Howard wave function, $k_{F}^{i} = \sqrt{2\pi n^{i}}$ is the Fermi wave vector, and $d$ is the distance between carriers and surface charged impurities.

2. Acoustic phonon scattering

Phonon is a quantum of lattice vibration and causes carrier scattering. There are two modes in the lattice vibrations: acoustic and optical modes. The room-temperature mobility of diamond is mainly affected by acoustic phonons\textsuperscript{[8]}. The scattering rate caused by acoustic phonon is given by

$$
\frac{1}{\tau_{\text{ac}}^{i}} = \frac{3m_{\text{eff}}^{i} k_{B} T D_{\text{ac}}^{2}}{16\rho u_{l}^{2} \hbar^{5}}. \quad (12)
$$

$D_{\text{ac}}$ is the acoustic deformation potential, $\rho$ is the crystal mass density, and $u_{l}$ is the velocity of longitudinal acoustic phonons. The deformation potential of diamond was calculated to be 8 eV by Cardona \textit{et al.} using the Linear combination of muffin tin orbitals (LMTO) method\textsuperscript{[14]} This value is consistent with the temperature dependence of mobility of boron-doped diamond in the study by Pernot \textit{et al.}\textsuperscript{[13]} $\rho$ and $u_{l}$ of diamond are 3515 kgm$^{-3}$ and 17536 ms$^{-1}$, respectively\textsuperscript{[13]}. 

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3. Surface roughness scattering

The surface roughness induces the disorder in the electric potential and leads to the carrier scattering. The scattering rate caused by the surface roughness is given by

$$\frac{1}{\tau_i} = \frac{\Delta^2 \Lambda^2 e^4 m_i^i}{(\epsilon_0 \epsilon_s)^2 \hbar^2 (n_{tot})^2} \int_0^1 u^4 \exp[-(k_F u)^2 \Lambda^2 u^2] \frac{u + G(b^i, q)q_{TF}/(2k_F)^2}{\sqrt{1 - u^2}} du. \quad (13)$$

The surface roughness is characterized by the average roughness ($\Delta$) and correlation length ($\Lambda$).

The total scattering rate is calculated using the Mathiessen rule,

$$\frac{1}{\tau_i} = \frac{1}{\tau_{imp}^i} + \frac{1}{\tau_{ac}^i} + \frac{1}{\tau_{r}^i}, \quad (14)$$

and the mobility for $i=\text{HH}, \text{LH}, \text{SO}$ is obtained from $\mu^i = e\tau_i^i/m_i^i$. We finally calculated the carrier density and mobility of the FET using the formula for the multi-carrier Hall effect, because our experimental results are obtained from low magnetic field Hall effect measurements.

$$\mu = \frac{n^{\text{HH}}(\mu^{\text{HH}})^2 + n^{\text{LH}}(\mu^{\text{LH}})^2 + n^{\text{SO}}(\mu^{\text{SO}})^2}{n^{\text{HH}}\mu^{\text{HH}} + n^{\text{LH}}\mu^{\text{LH}} + n^{\text{SO}}\mu^{\text{SO}}}, \quad (15)$$

$$n = \frac{(n^{\text{HH}}\mu^{\text{HH}} + n^{\text{LH}}\mu^{\text{LH}} + n^{\text{SO}}\mu^{\text{SO}})^2}{n^{\text{HH}}(\mu^{\text{HH}})^2 + n^{\text{LH}}(\mu^{\text{LH}})^2 + n^{\text{SO}}(\mu^{\text{SO}})^2}. \quad (16)$$

### III. RESULTS AND DISCUSSION

Figure 2 shows the carrier density dependence of mobility of our three diamond FETs with a h-BN gate dielectric. The figure also shows the mobilities of diamond FETs reported by other groups and the mobility of surface conductivity of hydrogen-terminated diamond surfaces exposed to air. The mobilities of our FETs exceed 300 cm$^2$V$^{-1}$s$^{-1}$, and they are only weakly dependent on the carrier density. This contrasts with the mobilities of the surface conductivity induced by the air exposure, which decreases monotonically with carrier density.

Here let us consider which scattering mechanism limits the mobility of our FETs. The carrier density dependence of the mobility limited by acoustic phonon scattering can be calculated only using material-dependent parameters such as the deformation potential and phonon velocity. As shown in Fig. 2, the calculated acoustic-phonon-limited mobility is more than one order of magnitude higher than the experimental one, and therefore, acoustic...
phonon is not the dominant scattering source in our FETs. The high acoustic-phonon-limited mobility is due to the high phonon velocity and the large crystal mass density in diamond.

The analytical formula for the surface roughness scattering contains device-dependent parameters, $\Delta$ and $\Lambda$, which characterize the magnitude of surface roughness. Here, we assume $\Delta = 0.3$ nm and $\Lambda = 2$ nm. The validity of these values is described below. The calculated mobility limited by the surface roughness scattering is also higher than the experimental one, and it is a strongly decreasing function of carrier density. Therefore, the surface roughness scattering cannot explain the overall behavior of the mobility of our FETs, either.

The surface impurity scattering with a constant impurity density leads to a slow increase of the mobility with carrier density if the distance between the impurities and the two-dimensional hole gas is small. (Fig. 3) We calculate the mobility limited by surface charged impurities for different $n_{\text{imp}}$ by assuming $d = 0$. The total mobility calculated with $n_{\text{imp}} = (0.8-1.3) \times 10^{12}$ cm$^{-2}$ agrees reasonably well with the experimental mobility as shown in Fig. 2. The comparison between the experimental and calculated mobilities indicates that the surface impurity scattering is the dominant mechanism that limits the mobility of our FETs.

We assumed $\Delta=0.3$ nm and $\Lambda=2$ nm for the calculation of surface roughness scattering rate as described above. Taking different values of $\Lambda$ does not influence the carrier density dependence of mobility considerably for the carrier density lower than $5 \times 10^{12}$ cm$^{-2}$ (Fig. 4(a)). $\Lambda = 2$ nm is the same as that obtained by Li et al. from the comparison between experimental data and calculations. This value is also comparable with those used for explaining the mobility in a Si MOSFET$^{15}$ and an AlGaN/GaN heterostructure$^{16}$. The value of $\Delta$, in contrast, affects the carrier density dependence of the mobility significantly as shown in Fig. 4(b). If $\Delta$ is larger than 1 nm, mobility decreases rapidly with increasing carrier density. Such a rapid decrease is inconsistent with the experimental results. The experimental mobility can be explained most reasonably with $\Delta \approx 0.3$ nm. This is within a typical range of the surface roughness of polished diamond substrates.

As shown in Fig. 2 the calculated mobility of heavy holes ($\mu^{\text{HH}}$) is almost the same as the total mobility ($\mu$) calculated from Eq. (15), indicating the dominant role of heavy holes in the carrier transport. This is reasonable because the proportion of the density of heavy
holes is the largest and their effective mass parallel to the surface is the lightest.

We also examined the mobility of the surface conductivity of the hydrogen-terminated surface exposed to air. The monotonic decrease in mobility with increasing carrier density (Fig. 2) can be explained nearly quantitatively by the surface impurity scattering with \( n_{\text{imp}} = n_{2D} \), as was reported by Li et al.\(^8\). As the increase in carrier density means the increase in the density of charged impurities, the mobility monotonically decreases with carrier density. In the carrier density range between \( 10^{11} \) and \( 10^{14} \) cm\(^{-2}\), the surface impurity scattering leads to the lower mobility than those limited by acoustic phonon and surface roughness; therefore, the surface impurity scattering is dominant. We note that our calculation is performed using the effective masses for (111) surface, although Fig. 2 also shows the experimental results for both (100) and (111) surfaces. The difference in calculated mobility between (100) and (111) surfaces is less than 30\% and is within the variation of the experimental mobilities. We also note that the contribution of \( N_{\text{depl}} \) is not considered here; more accurately, \( n_{\text{imp}} \) should equal \( n_{2D} + n_{\text{depl}} \) (\( n_{\text{depl}} = N_{\text{depl}} z_{\text{depl}} \), where \( z_{\text{depl}} \) is the depletion-layer thickness). We do not know \( n_{\text{depl}} \) in the diamond samples in the literature from which the mobility of the surface conductivity are taken for Fig. 2. The above Schrödinger-Poisson calculations show that \( n_{\text{depl}} = 7 \times 10^{11} \) cm\(^{-2}\) for \( N_{\text{depl}} = 1.76 \times 10^{16} \) cm\(^{-3}\) (0.1 ppm) and \( n_{\text{depl}} = 2.3 \times 10^{12} \) cm\(^{-2}\) for \( N_{\text{depl}} = 1.76 \times 10^{17} \) cm\(^{-3}\) (1 ppm). If \( n_{\text{depl}} \) is taken into account, the calculated mobility for \( n_{2D} \ll n_{\text{depl}} \) is lower than that shown in Fig. 2 because \( n_{\text{imp}} \approx n_{\text{depl}} \) for \( n_{2D} \ll n_{\text{depl}} \).

The above comparison between the experimental and calculated mobility indicates that the surface impurity scattering is the dominant mechanism that limits the mobility of our FETs. This is consistent with our recent finding that the quantum and transport lifetime, which are estimated from Shubnikov-de Hass oscillations at low temperatures, are nearly the same.\(^{17}\) The surface charged impurities may be adsorbed when the diamond surface is exposed to air before it is laminated by a flake of h-BN.\(^{10}\) Most of the heterostructures consisting of graphene and h-BN are also created by stacking the layers with their surfaces exposed to air. The interfaces of the layers can nevertheless be free from the adsorbates due to a unique self-cleansing effects.\(^{15}\) However, such self-cleansing effects seem to be ineffective for the interface between the hydrogen-terminated diamond and h-BN. For improving the mobility of the FETs, it would be important to reduce the density of adsorbates, for example, by a vacuum annealing.\(^{10}\) As shown in Fig. 2, our calculation suggests that decreasing the
density of charged impurities down to $\approx 1 \times 10^{11}$ cm$^{-2}$ would lead to the mobility above 1000 cm$^2$V$^{-1}$s$^{-1}$ at room temperature. The surface roughness scattering should also be reduced for improving the mobility for carrier densities higher than $\approx 4 \times 10^{12}$ cm$^{-2}$. For this purpose, it will be effective to use the atomically flat diamond surface prepared by the chemical vapor deposition with a low methane concentration on a mesa structure.$^{20,21}$

IV. CONCLUSIONS

In conclusion, we calculated the carrier density dependence of mobility of hydrogen-terminated diamond FET considering three scattering mechanisms: the surface impurity scattering, acoustic phonon scattering, and surface roughness scattering. The calculated mobility agrees with the mobility of our diamond FETs with a h-BN gate dielectric if we assume a constant surface impurity density $n_{\text{imp}} = (0.8 - 1.3) \times 10^{12}$ cm$^{-2}$, an average surface roughness $\Delta = 0.3$ nm and a correlation length $\Lambda = 2$ nm. Decreasing the surface impurity density below $\approx 1 \times 10^{11}$ cm$^{-2}$ will lead to a mobility exceeding 1000 cm$^2$V$^{-1}$s$^{-1}$. Such a high mobility outperforms that of $p$-type Si MOSFET significantly and will be useful for developing electronic devices that operate with a low loss and a high speed.

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FIG. 1. (a) The calculated density profile of the lowest subbands of heavy- (HH), light- (LH), and split-off (SO) holes and the 2nd subband of heavy holes (HH2) for the total carrier density of $1.0 \times 10^{13} \text{cm}^{-2}$ at $T = 300$ K. $z$ is the depth from the diamond surface. $N_{\text{depl}}$ is assumed to be 0.5 ppm. (b) The calculated population of heavy holes, light holes, and split-off holes as a function of total carrier density at $T = 300$ K.
FIG. 2. The carrier density dependence of mobility. Solid lines show the calculated results for hydrogen-terminated diamond FET. Dotted lines show the calculated results for the surface conductivity of hydrogen-terminated diamond. The figure also shows that the experimental results\textsuperscript{[10]} of our h-BN/diamond FETs, other group’s diamond FETs and surface conductivities. Squares, circles, and triangles represent (111), (100), and (110) diamond surfaces, respectively. The rhombus represents a polycrystalline diamond.

FIG. 3. The calculated carrier density dependence of mobility limited by surface impurity scattering. The density of surface charged impurity $n_{\text{imp}}$ is $1.3 \times 10^{12}$ cm$^{-2}$. $d$ is the distance between the charged impurities and the two-dimensional hole gas.
FIG. 4. (a) The calculated carrier density dependence of mobility for different $\Lambda$ values. Here, $\Delta$ is 0.3 nm and $n_{\text{imp}}$ is $1.3 \times 10^{12}$ cm$^{-2}$. (b) The calculated carrier density dependence of mobility for different $\Delta$ values. $\Lambda$ is 2 nm and $n_{\text{imp}}$ is $1.3 \times 10^{12}$ cm$^{-2}$. 