Impact of Space-Energy Correlation on Variable Range Hopping in a Transistor

J.-F. Morizur,[1] Y. Ono,[1,*] H. Kageshima,[1] H. Inokawa,[2] and H. Yamaguchi[1]
[1]NTT Basic Research Laboratories, NTT Corporation, 3-1 Morinosato Wakamiya, Atsugi, Kanagawa 243-0198, Japan
[2]Research Institute of Electronics, Shizuoka University, 3-5-1, Johoku, Hamamatsu, 432-8011, Japan
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Hopping conduction *in transistors*, i.e., under a transverse electric field, is addressed using percolation theory with a space-energy correlation in the density of states of the impurity band. The computation of the percolation threshold over an extended range of correlation parameters enables us to derive a formula, which, while giving the classical results in the low field limit, describes the emergence of a specific variable range hopping in the high field case. An application of this formula to experimentally extract the localization radius is also proposed.

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Hopping [1,2] has been one of the central issues of charge transport and, recently, attracts renewed attention from viewpoints of future nano/quantum information processing, a part of which requires a deep understanding of hopping (or tunneling) via impurity levels in field-effect transistors [3]. Percolation theory [1] applied to disordered systems has proved powerful in describing the conduction characteristics of hopping phenomena. This theory has shown that the density of states (DOS) properties, such as spatial dimension, energy bandwidth, and strength of the Coulomb interaction, which can create a gap in the DOS around the Fermi energy, have direct influences on conduction characteristics such as temperature and concentration dependence [4,5]. However, the existing theory is not applicable for a situation with transverse electric field despite its great importance already demonstrated by some experimental studies using transistors [6–8].

Here, we investigate the hopping transport in a high transverse field based on the percolation theory with a correlation between the spatial and energy dimensions, and show that the hopping properties in transistors are qualitatively different from the ones in ordinary bulk materials. After presenting the necessary framework of percolation theory, we show that a nonzero gradient in the average energy of sites significantly reduces the effect of the Coulomb interaction on the DOS. Then, we show the results of the computations and derive a physically meaningful formula for the percolation threshold. This formula predicts the transition from a three-dimensional (3D) to a specific two-dimensional (2D)-like hopping as the gradient of energy is increased. We also propose, on the basis of these results, a new experimental method to determine the localization radius of carriers in localized states.

Miller and Abrahams' model [9] is used to derive probability P_{ij} that one electron jumps from one site to another. This probability can be written as $P_{ij} \propto \exp(-\xi_{ij})$, where $\xi_{ij} = \frac{2R_{ij}}{a_0} + \frac{\varepsilon_{ij}}{kT}$ if the wave function of the charge is isotropic. Here, R_{ij} is the distance between the two sites, a_0 the localization radius, and ε_{ij} can be expressed as $\varepsilon_{ij} = \frac{1}{2}(|\varepsilon_i - \mu| + |\varepsilon_j - \mu| + |\varepsilon_i - \varepsilon_j|)$, with μ the Fermi energy, ε_i and ε_j the energy of site i and j, respectively [10]. To compute the total resistance of the network, percolation theory can be used [1]. It involves finding the percolation threshold ξ_c. For a certain dimensionless $\xi_{\rm opt}$, one can consider the networks of sites created under the condition $\xi_{ij} < \xi_{\rm opt}$ for all pairs of i and j. The ξ_c is the smallest $\xi_{\rm opt}$ that allows a network of sites to become infinite. Percolation theory simply yields the results that the conductivity of the network is proportional to $\exp(-\xi_c)$. Computing ξ_c is possible in a "dimensionless space", which is a 4D (one energy and three spatial coordinates) space with dimensionless variables. We introduce a length scale $R_{\rm opt} = \frac{a_0 \xi_{\rm opt}}{2}$ and an energy scale $\varepsilon_{\rm opt} = kT\xi_{\rm opt}$, and then the bonding criterion $\xi_{ij} < \xi_{\rm opt}$ is expressed as $s_{ij} + e_{ij} < 1$. The spatial term is $s_{ij} = ||\vec{s}_i - \vec{s}_j||$ with $\vec{s}_i = \frac{\vec{R}_i}{R_{\rm opt}}$. The energy term is $e_{ij} = \frac{1}{2}(|e_i| + |e_j| + |e_i - e_j|)$ with $e_i = \frac{\varepsilon_i - \mu}{\varepsilon_{\rm opt}}$. The only sites able to bond are the sites at which $|e_i| < 1$, which is a necessary condition for the bonding criterion and thus can be used as a boundary condition when solving the problem.

If we consider that the DOS around the Fermi energy is a constant $g(\mu)$, i.e., the case of Mott's variable range hopping (VRH), the number of sites $N(\xi_{\rm opt})$ in a cube of side A in the dimensionless space with $|e_i| < 1$ is

$$N(\xi_{\rm opt}) = A^3 2g(\mu)\varepsilon_{\rm opt}{R_{\rm opt}}^3 = A^3 \frac{1}{4} g(\mu)kT{a_0}^3{\xi_{\rm opt}}^4. \quad (1)$$

We compute $N(\xi_{\rm opt}) = N_c$ necessary in the dimensionless cube of side A with $|e_i| < 1$ to reach percolation [1]. As a result, we find $\xi_c = (\frac{4n_c}{{a_0}^3 kTg(\mu)})^{1/4}$, where $n_c = \lim_{A\to\infty} \frac{N_c}{A^3}$ is called the critical concentration [1], at which percolation first occurs. The same kind of computation can be done in the 2D case, which yields

$$\xi_c = \left(\frac{2\tilde{n}_c}{a_0^2 kT\tilde{g}(\mu)}\right)^{1/3}, \quad (2)$$

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where $\tilde{n}_c = \lim_{A\to\infty} \frac{\tilde{N}_c}{A^2}$ is the (2D) critical concentration and $\tilde{g}(\mu)$ is the 2D DOS [11]. In order to accept the DOS constant, the condition $w \gg 2kT\xi_c$, with w the typical width of the DOS, must be true [4]. The above derivations are thus done considering that w is infinite.

Let us now focus on our specific model $g_{\rm sp}$ for a DOS, which is presented in the inset of Fig. 2(a). We introduce a gradient in the energy of sites, which is set perpendicularly to the electron flow, in order to respect the linear response theory at the base of the Miller Abrahams' model. We assume that this gradient is constant. To that extent, we consider the simple DOS $g_{\rm sp}(\varepsilon, z) = g_0$ on the range $|\varepsilon - cz| < w/2$ and $g_{\rm sp}(\varepsilon, z) = 0$ outside, where c is the slope of the variation of the average of the energy with z. Comparing this model to a real DOS, such as that for an impurity band, w accounts for the energy bandwidth while c represents the energy shift resulting from a nonzero transverse electric field. Introducing a finite bandwidth w makes our model more general than the constant-DOS models previously discussed above, since our model is not limited by the condition $w/2 \gg kT\xi_c$. The structure of $g_{\rm sp}$ introduces a linear correlation between the two random variables ε_i and z_i. Parameter c is the average ratio $\langle \varepsilon_i/z_i \rangle$, while parameter w (or equivalently w/c) defines the strength of the correlation between the two variables. In the limit case when $w \to 0$, the position of a site along the z axis gives directly its energy $\varepsilon_i = cz_i$. In such a case, we will observe a strong dependence of the percolation threshold upon c. As w is increased, this dependence will be reduced.

The above $g_{\rm sp}$ is assumed to be constant around the Fermi energy at $z = 0$. Before exhibiting the computation results of the percolation threshold, we must explain why this simple DOS is coherent with the Coulomb interaction issue. According to Refs. [5,12], the Coulomb interaction leads to a modification of the DOS in order to ensure that, for any given pair of sites i and j, with $\varepsilon_i > \mu > \varepsilon_j$, the condition, $\varepsilon_i - \varepsilon_j - \frac{q^2}{4\pi\kappa R_{ij}} > 0$, stands true, where q is a unit of charge and κ the permittivity. This condition implies a vanishing of the DOS for energies close to the Fermi energy, and at first sight contradicts our model DOS. Let us explain on which conditions the constant DOS around the Fermi energy is relevant. The above condition with our specific $g_{\rm sp}$ is necessarily fulfilled for sites that are far enough away on the z axis. The relations $\varepsilon_i > cz_i - w/2$ and $\varepsilon_j < cz_j + w/2$ give the sufficient condition, $c(z_i - z_j) - w - \frac{q^2}{4\pi\kappa R_{ij}} > 0$. If we consider the average distance R_d to the closest site, the average distance on the z axis to the closest site is $R_d/\sqrt{3}$, considering that the spatial distribution of sites is random and isotropic. As a result, the following condition for c allows us to neglect the Coulomb gap in the DOS: $c\frac{R_d}{\sqrt{3}} \gg \frac{q^2}{4\pi\kappa R_d} + w$. It is easily satisfied. For example, considering impurity conduction in a doped Si with a doping density of $N_d = 9.0 \times 10^{17}$ cm^{-3} and $w = 10$ meV [13], the condition can be written as $c \gg 3.6$ meV/nm, which is achievable in experimental conditions, if the Si is put in a transistor structure [8].

To visualize this analytical condition, a small computation work was performed, and the results are shown in Fig. 1. We considered 10 000 randomly distributed sites in a cube with 220-nm sizes, which gives a density of $N_d = 9.0 \times 10^{17}$ cm^{-3}. Their energy is random on a band of width $w = 10$ meV. We then checked, among all the possible pairs in the sample, which ones should not exist, i.e., which ones do not respect the condition, $\varepsilon_i - \varepsilon_j - \frac{q^2}{4\pi\kappa R_{ij}} > 0$. For every pair that does not respect the condition, one (chosen randomly) of the two concerned sites is deleted. Although this is not a complete process for determining the DOS, which requires a self-consistent calculation, this method still gives an idea of the extent of the influence of the Coulomb interaction on the DOS. The remaining number of sites, which constitute a physically consistent DOS, is presented in Fig. 1(a). We then increased the slope, keeping the impurity bandwidth constant. This gives the results in Figs. 1(b)–1(d), for slopes of 0.1, 1.0, and 4.0 meV/nm, respectively. The physical meaning of the disappearance of the gap is simple: under a high electric-field, the condition $\varepsilon_i - \varepsilon_j - \frac{q^2}{4\pi\kappa R_{ij}} > 0$ is rarely violated even for two sites close to each other. The conclusion from this calculation is that the Coulomb gap can effectively be neglected if the condition, $c\frac{R_d}{\sqrt{3}} \gg \frac{q^2}{4\pi\kappa R_d} + w$, is respected.

We now show the computational results for the percolation threshold. Our specific DOS $g_{\rm sp}$ translates in the dimensionless space into a constant DOS on the range $|e_i - Cs_{iz}| < W \cap |e_i| < 1$ and null outside this range. The dimensionless coefficients C and W have the form $C = \frac{ca_0}{2kT}$ and $W = \frac{w}{2kT\xi_{\rm opt}}$. We consider $0 < s_{ix,y} < A$, and the boundary condition for s_{iz} is implicitly included in $|e_i - Cs_{iz}| < W \cap |e_i| < 1$. We then compute the necessary $N_c(C, W)$ for $A = 7$ in order to reach percolation [14].

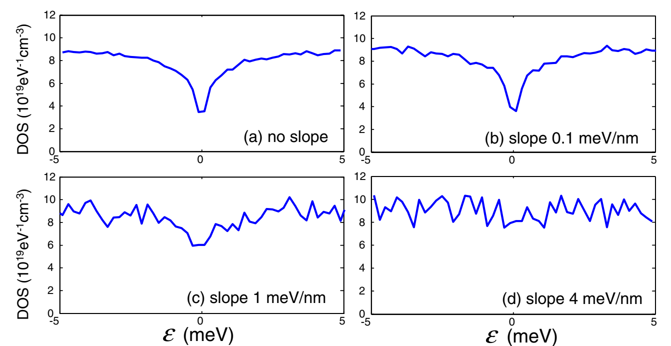

FIG. 1 (color online). Computed DOS. A clear Coulomb gap is observed in (a) while it is barely perceivable in (d).

The results are averaged over 40 realizations for each value of C and W (Figs. 2 and 3.). Notice that $N_c(C, W)$ with $0 < s_{ix,y} < A$ is given by $N_c(C, W) = 2A^2 R_{\text{opt}}(\xi_c)^2 \varepsilon_{\text{opt}}(\xi_c) \times \frac{w}{c} g_0 = A^2 a_0{}^2 \xi_c{}^3 kT \frac{w}{2c} g_0$. This is a function of parameters C and W, and, to that extent, strongly differs from Eq. (1).

We propose a physically meaningful formula to understand the raw data produced by the computation. Considering

$$\frac{N_c(C, W)}{A^2} = \gamma_1 \frac{W}{C} + \gamma_2 \frac{1}{C} + \gamma_3 \frac{\sqrt{W}}{C} + \gamma_4, \qquad (3)$$

which is equivalent to $a_0{}^3 \xi_c^4 kT g_0 = 2\gamma_1 + 4\gamma_2 \frac{kT\xi_c}{w} + 2\sqrt{2}\gamma_3 (\frac{kT\xi_c}{w})^{1/2} + 2\gamma_4 \frac{ca_0\xi_c}{w}$, a fitting was performed in parallel on the two ranges exhibited in Figs. 2(b) and 3 in order to derive the numerical coefficients γ_i. This fitting procedure yields $\gamma_1 = 4.8$ $\gamma_2 = 1.0$, $\gamma_3 = -1.3$, $\gamma_4 = 4.3$.

In what follows, we thoroughly analyze the above formulation. First, the low-slope limit case ($C \ll 1$) can be understood using classical results for hopping in no-slope situation. In Mott's VRH case, i.e., on the condition $W \gg 1$, direct computation yields $\xi_c = (\frac{10.0}{a_0{}^3 kT g_0})^{1/4}$, while our formulation fitted on our computed data gives $\xi_c = (\frac{9.7}{a_0{}^3 kT g_0})^{1/4}$. Mott's VRH is thus well described by our model, and the numerical coefficient is reproduced, even though no extrapolation for A infinite was performed. In the nearest neighbor hopping (NNH) case [15], i.e., for $W \ll 1$, while direct computation gives $\xi_c = (\frac{3.2}{a_0{}^3 N_d})^{1/3}$, we extract $\xi_c = (\frac{4.0}{a_0{}^3 N_d})^{1/3}$, again reflecting this limit case. The third important term in the low-slope limit is $-3.6(\frac{kT\xi_c}{w})^{1/2}$. This term accounts for the gradual transition [4] between the two limit cases, $W \ll 1$ and $W \gg 1$, in the low-slope situation. Indeed, this term cannot be neglected only when $W \approx 1$ with regards to W and 1. To that extent, it introduces a correction on the transition range from Mott's VRH to NNH and this is why only this term has a negative coefficient. The three discussed terms account for the terms $\gamma_1 \frac{W}{C} + \gamma_2 \frac{1}{C} + \gamma_3 \frac{\sqrt{W}}{C}$ in Eq. (3). No higher order in $1/C$ is possible, since it would be dominant when C tends to 0 and would not reflect the classical results for Mott's VRH and NNH. Figure 2(a) shows the particular linear dependence of N_c/A^2 in $1/C$.

We next study the high-slope case, $C \gg 1$ and $C \gg W$. The computation results, exhibited in Fig. 3(a), strongly suggest that a constant must be added to $\gamma_1 \frac{W}{C} + \gamma_2 \frac{1}{C} + \gamma_3 \frac{\sqrt{W}}{C}$ in Eq. (3) to reproduce the offset observed there. Terms with smaller exponent in C (i.e., with a power law of C^o, where $-1 < o < 0$) could be introduced in Eq. (3) to allow for more precise fitting, but the already sufficiently good fitting of the computation results indicates that these corrections are small. Indeed, if we consider the computed values of N_c/A^2 for C higher than 5 and smaller than 0.2, the average relative error is 4%, while, if we consider our whole computation space, the average relative error is 8%. Since N_c/A^2 is obviously a constant in the high-C limit, higher orders in C are not allowed in the formula by our computation results. As a conclusion, Eq. (3) has a strong physical background in the low-slope case, and also clearly indicates the existence of an additional term in the general case.

Let us now discuss in more detail this new term found in our percolation threshold. In the high-slope case of $C \gg 1$ and $C \gg W$, the constant term in Eq. (3) gives

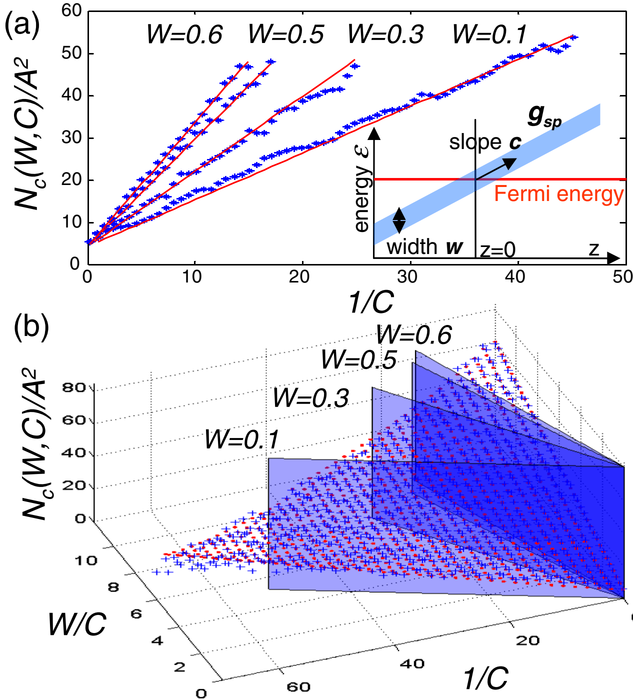

FIG. 2 (color online). Computation results for a wide range of $1/C$. (a) N_c/A^2 against $1/C$, extracted for constant W's. Dots are computation results and lines are values from Eq. (3). The position of the planes where W is constant is shown in (b). (b) N_c/A^2 against W/C and $1/C$. Crosses are computation results and dots are values from Eq. (3). The planes of constant W for (a) are exhibited. Inset in (a): Model DOS $g(\varepsilon, z)$. The current flows perpendicularly to the page.

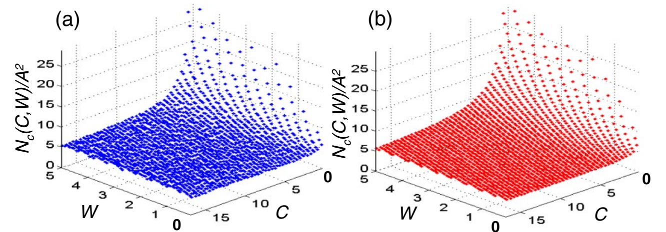

FIG. 3 (color online). Computation results for N_c/A^2 against C and W, for the high-slope limit. (a) Computation results and (b) values extracted from Eq. (3). An offset in N_c/A^2 is visible.

$$\xi_c = \left(\frac{8.5c}{a_0{}^2 kTN_d}\right)^{1/3}, \quad (4)$$

where $N_d = g_0 w$ is the site density, and the coefficient 8.5 can be interpreted as a critical concentration in this limiting case. The $1/3$ exponent, in contrast to an ordinary $1/4$, is seen as the collapse of the correlated spatial and energy dimensions together. That is why Eq. (4) is similar to the result of a 2D percolation problem, Eq. (2). Still, fundamental differences from 2D VRH are observed.

First, the temperature range is modified. Indeed, in 2D VRH, the condition for the observation of the $1/3$ exponent in the temperature-dependence is $w \gg 2kT\xi_c$. Here, the conditions are $w \ll ca_0\xi_c$ and $kT \ll ca_0$. Fundamentally, what happens is that the limitation introduced by a finite bandwidth disappears due to its stretching by the slope. At the same time, the energy boundary $kT\xi_c$ for the participating states in the hopping process is introduced in the lateral displacement along the z axis. Thus, the spatial dimension z and the energy scale ε collapse together, sharing their properties and giving way to a 2D-like hopping temperature dependence.

Even more important is the difference in the dependence on the DOS shape. In the case of no-slope 2D VRH [1,11], according to Eq. (2), the percolation threshold strongly depends upon $\tilde{g}(\mu)$. In the case of a high slope, the percolation threshold, Eq. (4), only depends on the site density N_d and on the slope c. Indeed, for high slopes, the energy difference between two sites will be dominated by the difference induced by the slope. To that extent, the actual shape of the energy dependence of the DOS will be of small importance, since the slope will tend to average it. That is why, in the case of high slopes, the energetic shape of the DOS is not important, and computing the percolation threshold for any other shape with the same typical width w would give the exact same result in the high-slope limit.

The independence of the percolation threshold on the shape of the DOS is of tremendous importance in experimental applications, especially in the evaluation of the localization radius, since determining the precise energy dependence of the DOS of the impurity band is difficult, whereas the mere extraction of N_d can be done by many means [16]. If we consider impurity hopping in a field-effect-transistor structure [8], with enough gate bias so that the transverse electric field induced gives $kT \ll ca_0$ and $w \ll ca_0\xi_c$, a_0 can be expressed as $a_0{}^2 = 2\gamma_4 \frac{\partial c}{\partial V} \times (N_d \frac{\partial T_0}{\partial V})^{-1}$, where V is the gate bias and T_0 a characteristic temperature derived from temperature-dependence measurement. A precise calculation of $\frac{\partial c}{\partial V}$ is possible [8,17], allowing an accurate extraction of a_0. This method gives a new and simple experimental way to measure the localization radius without the need to progressively add layers of matter to the sample as was done in [18]. The above two conditions $w < ca_0\xi_c$ and $kT < ca_0$ will both be met at 10 K in a buried-channel silicon-on-insulator (SOI) field-effect transistor [8] doped with phosphorus by $N_d \sim 10^{18}$ cm^{-3}, for a voltage difference of 40 meV on a SOI thickness of 10 nm.

In summary, the correlation between the energy of a site and its position, such as induced by an electric field, changes the fundamental properties of hopping transport in semiconductors. The merging of the spatial and energy coordinates modifies the temperature dependence and makes the conduction insensitive to the DOS structure. This predicts the different behaviors for hopping in field-effect transistors from that in a bulk semiconductor and suggests a new way to derive experimentally the localization radius of the impurity electrons.

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*Corresponding author.
Electronic address: ono@aecl.ntt.co.jp

[1] B. I. Shklovskii and A. L. Efros, *Electronic Properties of Doped Semiconductors* (Springer-Verlag, Berlin, 1984).
[2] N. F. Mott and E. A. Davis, *Electronic Processes in Non-Crystalline Materials* (Clarendon, Oxford, 1979); N. F. Mott, J. Non-Cryst. Solids **1**, 1 (1968); M. Pollak and B. I. Shklovskii, *Hopping Transport in Solids* (North-Holland, Amsterdam, 1991).
[3] S. Kumar *et al.*, Phys. Rev. Lett. **95**, 066802 (2005); J. H. Cole *et al.*, Phys. Rev. B **71**, 115302 (2005); L. C. L. Hollenberg *et al.*, Phys. Rev. B **69**, 113301 (2004).
[4] M. Pollak *et al.*, Phys. Rev. Lett. **30**, 856 (1973).
[5] A. L.Efros and B. I. Shklovskii, J. Phys. C **8**, L49 (1975); A. L. Efros, J. Phys. C **9**, 2021 (1976).
[6] M. Pepper, Philos. Mag. B **37**, 187 (1978).
[7] A. B. Fowler *et al.*, Phys. Rev. Lett. **57**, 138 (1986).
[8] Y. Ono *et al.*, Phys. Rev. B **74**, 235317 (2006).
[9] A. Miller and E. Abrahams, Phys. Rev. **120**, 745 (1960).
[10] V. Ambegaokar *et al.*, Phys. Rev. B **4**, 2612 (1971).
[11] A. S. Skal and B. I. Schklowskii, Fiz. Tverd. Tela (Leningrad) **16**, 1820 (1974) [Sov. Phys. Solid State **16**, 1190 (1974)].
[12] M. L. Knotek and M. Pollak, Phys. Rev. B **9**, 664 (1974).
[13] R. N. Bhatt and T. M. Rice, Phys. Rev. B **23**, 1920 (1981).
[14] In our computation, the 3-ellipsoid structure of the donor wave function was taken into account. This new bonding criterion does not change the fundamental behaviors but rather allows for the computing of more precise parameters for a certain type of semiconductor including silicon.
[15] C. H. Seager and G. E. Pike, Phys. Rev. B **10**, 1435 (1974).
[16] Y. Ono *et al.*, Jpn. J. Appl. Phys. **44**, 2588 (2005); Y. Sato *et al.*, J. Electrochem. Soc. **142**, 660 (1995).
[17] S. Horiguchi *et al.*, Jpn. J. Appl. Phys. **43**, 2036 (2004).
[18] M. L. Knotek *et al.*, Phys. Rev. Lett. **30**, 853 (1973).