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Theory of electron transport in a two-dimensional layer on the solid hydrogen surface

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The mobility of electrons localized over solid hydrogen is investigated theoretically using the Boltzmann equation. It is shown that the electron mobility for temperatures above 5 K is dominated by the interface roughness scattering of the hydrogen surface, which is described by the two-parameter model of Gaussian correlations. From detailed comparison between theory and experiment it is determined that the hydrogen surface has a roughness with the height of about 1–2 atomic sizes and a lateral width in the mesoscopic scale (about 10^{-6} cm). The theoretical dependences of the mobility on the temperature obtained are in excellent agreement with the experimental high-temperature data available. However, for temperatures below 5 K, our results reproduce only qualitatively the overall temperature dependence of the mobility.

I. INTRODUCTION

Even though Cole and Cohen[1] have predicted that two-dimensional electrons are also possible on the surface of solid hydrogen and neon, as in liquid helium, Troyanovskii, Volodin, and Khaikin[2] demonstrated, 15 years ago, that electrons are actually localized on the surface of these materials. At the present time, the systems of electrons over solid hydrogen and neon are practically the only realized examples of the electron localization in a two-dimensional layer near a dielectric surface in addition to the well-known electron localization over the liquid helium surface. Experiments with electrons on bulk hydrogen were reported by Troyanovskii and Khaikin,[3] who measured the ac conductivity of the surface electrons, by Edel'man and Faley,[4] who made cyclotron resonance studies, and by Cieslikowski and co-workers[5,6] who measured the mobility at low frequencies. Kajita[7,8] had performed a systematic study of surface electrons on solid neon. The scattering mechanisms for the surface electrons are vapor molecules, surface excitations (Rayleigh waves in the case of solid substrate and ripplons in the case of liquid helium), and surface defects. In the case of solid hydrogen, whose dielectric constant $\varepsilon_H = 1.29$ (for helium $\varepsilon_{He} = 1.057$), the mean distance of the electron from the hydrogen surface in the ground state $\langle z \rangle_1 = 24$ Å , while for the surface of bulk liquid helium this distance is 114 Å. For this reason the influence of the surface roughness on the properties of the localized electron over hydrogen is much more pronounced than in the case of liquid helium. This influence was registered experimentally by Troyanovskii and Khaikin [3] and by Edel'man and Faley[4] at temperatures $T < 12$ K. Both experiments demonstrated that the scattering by surface defects is the main mechanism determining the electron mobility in this temperature range, since the gas atom scattering becomes extremely small and the mobility due to the scattering from Rayleigh waves, as calculated in Ref. 3, exceeds the experimental data by more than two orders of magnitude. The experimental values of the electron mobility obtained in Refs. 3 and 4 are close. However, the interpretation of the results obtained is quite different. According to Ref. 3, the mobility is determined by electron scattering from microscopic surface defects with characteristic dimensions of 5×10^{-8} cm. Edel'man and Faley[4] concluded that their results can be explained only if the solid hydrogen surface can be represented by some kind of terrace structure with the size of flat sections about 10^{-5} cm and steps much larger than an atomic distance.

The difficulties in the interpretation of the influence of the hydrogen surface roughness on the kinetic properties of the electron system lead to numerous investigations of the effects which arise when the hydrogen surface is covered by a superfluid helium film. This covering, resulting in the smoothing of the surface defects, influences strongly the electron properties and interesting results are obtained both experimentally and theoretically.[9–12] Otherwise the experimental results on the electron mobility over the surface of hydrogen without covering are not explained up to present time, to our knowledge. Furthermore, the theoretical interpretation of these results can give not only the correct temperature dependence of the electron mobility observed but also the information about hydrogen surface defects whose values of characteristic heights and longitudinal sizes are fitted directly in the calculation of the mobility.

The purpose of the present work is to investigate theoretically the mobility of the electrons localized over a solid hydrogen surface in the temperature range $1 < T < 10$ K. From the comparison with the experimental results we may check the reliability of the proposed model of surface defects, which is used in our approach, and conclude about the roughness structure of the solid hydrogen surface.

The paper is organized as follows. In Sec. II, the procedure of the calculation of the electron mobility above the solid hydrogen surface is described. The results obtained are interpreted and compared with experiments in Sec. III. Finally, our conclusions are summarized in Sec. IV.

II. THEORETICAL FORMULATION

The structure of the surface states of the electrons localized near the surface of solid hydrogen is similar to that over liquid helium. The energy spectrum of an electron can be written as

$$E_{n,k} = \frac{\hbar^2 k^2}{2m} - \frac{\Delta_0}{n^2} , \tag{1}$$

where $\Delta_0 = m\Lambda^2/2\hbar^2$, with $\Lambda = e^2(\varepsilon_H - 1)\ /\ 4(\varepsilon_H + 1)$, equal to 158.6 K. The two-dimensional wave vector $\vec{k}$ is in the (x, y) plane, the z axis is in the direction normal to the hydrogen surface, and m and e are the electron mass and charge, respectively.

The energy gap between ground ($n = 1$) and first excited surface levels ($n = 2$) is about 120 K. For this reason at temperatures near 10 K we can neglect the probability of an electron to escape from the ground surface level and we may only consider the case $n = 1$.

In this state the electron wave function is

$$\Psi(\vec{r}, z) = \frac{1}{\sqrt{S}} e^{i\vec{k}\cdot\vec{r}} \chi_\perp(z) , \tag{2}$$

$$\chi_\perp(z) = 2\gamma^{3/2}\ z\ e^{-\gamma\ z} , \tag{3}$$

where $\gamma = m\Lambda/\hbar^2 \simeq 6 \times 10^6\ \text{cm}^{-1}$, $\vec{r} = (x, y)$, and S is the area of the surface.

If a driving electric field is switched on along the plane of the vacuum-solid hydrogen interface, the electronic states, given by Eq. (2), will determine in the Born approximation the structure of the collision integral relative to the electron scattering by surface defects, which is given by

$$\widehat{S}_{ed}\{f\} = \frac{2\pi}{\hbar S} \sum_{\vec{q}} |\xi_q|^2 |\langle 1|V_q(z)|1\rangle|^2 [f(\vec{k} + \vec{q}) - f(\vec{k})] \times \delta\left[\frac{\hbar^2}{2m}\left(|\vec{k} + \vec{q}|^2 - |\vec{k}|^2\right)\right] , \tag{4}$$

where $f(\vec{k})$ is the distribution function; ξ_q is the Fourier transform of the function $\xi(\vec{r})$ which determines the profile of the hydrogen surface due to defects localized at $z = \xi(\vec{r})$. In the absence of defects, the position of the surface is given by the equation $z = 0$. $V_q(z)$ describes the interaction between the electron and surface defects. From the energy conservation law, which is satisfied at elastic collisions, we obtain $q \leq 2k$. This means that at temperatures $T \leq 10$ K the wave numbers q which contribute to scattering are in the long-wavelength limit, $q \leq 10^6\ \text{cm}^{-1}$. Under this condition the interaction potential can be chosen in a manner similar to that potential which describes the interaction of the surface electrons on helium with long-wavelength displacements of the interface liquid vapor[13,14]

$$V_q(z) = \frac{\Lambda q}{z}\left[\frac{1}{qz} - K_1(qz)\right] + eE_\perp . \tag{5}$$

Here $K_1(qz)$ is the modified Bessel function of the second kind, $E_\perp$ is the holding electric field in the z direction. In experiments[3,4] the holding field was $E_\perp < 500$ V/cm and the corresponding electron density in the two-dimensional (2D) layer was $n_s = E_\perp/2\pi e \leq 5 \times 10^8\ \text{cm}^{-2}$. At such charge concentration the system is far from quantum degeneracy (Fermi energy is about 10^{-2} K) and the distribution function can be determined from the Boltzmann kinetic equation, which can be written as

$$\frac{\partial f}{\partial t} + \frac{e\vec{E}}{\hbar} \cdot \frac{\partial f}{\partial \vec{k}} = \widehat{S}_{ed}\{f\} . \tag{6}$$

The methods of solving this kinetic equation are standard, and the mobility can be calculated by using the formula[14–17]

$$\mu(T) = \frac{e}{m} \int_0^\infty \frac{x e^{-x} dx}{\nu_{ed}\left(\frac{\sqrt{2mT}}{\hbar} x^{1/2}\right)} , \tag{7}$$

and the frequency ν_{ed} of the electron collisions with surface defects can be written as

$$\nu_{ed}(k) = \frac{m}{\pi\hbar^3 k^2} \int_0^{2k} \frac{q^2 |\xi_q|^2\ |\langle 1|V_q(z)|1\rangle|^2 dq}{\sqrt{4k^2 - q^2}} , \tag{8}$$

with

$$\Big|\langle 1|V_q(z)|1\rangle\Big|^2 = \frac{\Lambda q^2}{2} \varphi\left(\frac{q}{2\gamma}\right) + eE_\perp , \tag{9}$$

where

$$\varphi(y) = -\frac{1}{1 - y^2} + \frac{1}{(1 - y^2)^{3/2}} \ln\left(\frac{1 + \sqrt{1 - y^2}}{y}\right) \quad \text{for} \quad y < 1$$

and

$$\varphi(y) = -\frac{1}{1 - y^2} - \frac{1}{(y^2 - 1)^{3/2}} \arcsin\left(\frac{\sqrt{y^2 - 1}}{y}\right) \quad \text{for} \quad y > 1 .$$

We must emphasize that if the holding field is different from zero, the parameter γ entering into the electron wave function, Eq. (3), is not given by the expression $\gamma = m\Lambda/\hbar^2$, but would be dependent on $E_\perp$. In this case the parameter of Eq. (3) must be calculated using a more complicated formula coming from a variational procedure.[18] We have taken it into account in our calculations. However, the difference between the variational parameter and γ is negligible at $E_\perp < 500$ V/cm. For liquid helium, where the corresponding Λ is considerable less than that for hydrogen, the deviation of the true parameter and γ can be essential at such $E_\perp$.

In order to calculate ν_{ed}, we should choose a model of surface defects describing the amplitude ξ_q. Following Prange and Nee[19] (see also the classical review paper on 2D systems by Ando *et al.*[20]), the defects are represented by a roughness interface which is assumed to be characterized by the height ξ_0 and the lateral length l of the Gaussian fluctuations of the interface and expressed by the autocorrelation function given in terms of an ensemble average as

$$\langle \xi(\vec{r})\, \xi(\vec{r})\rangle = \xi_0^2 \, \exp\left(-\frac{|\vec{r}-\vec{r}|^2}{l^2}\right) , \tag{10}$$

which leads to

$$\left\langle |\xi_q|^2 \right\rangle = \pi \xi_0^2 l^2 \exp\left(-\frac{q^2 l^2}{4}\right) . \tag{11}$$

In the approximations described by Eq. (11) and Eq. (7) the mobility results as

$$\mu(T) = \frac{e\hbar^5}{32 m^3 \Lambda^2 \xi_0^2 T} \int_0^\infty \frac{x e^{-x} dx}{x F_1(k_T\, l\sqrt{x}) + \sqrt{x} F_2(k_T\, l\sqrt{x}) + F_3(k_T\, l\sqrt{x})} , \tag{12}$$

where $k_T = \sqrt{2mT}/\hbar$. The expressions for the functions $F_1(b)$, $F_2(b)$, and $F_3(b)$ are explicitly given by

$$F_1(b) = b^2 \int_0^{\pi/2} \sin^6(\theta)\, \varphi^2\left(\frac{b\sin(\theta)}{\gamma l}\right) e^{-b^2\sin^2(\theta)}\, d\theta , \tag{13}$$

$$F_2(b) = \frac{E_\perp \gamma l}{E_p} b \int_0^{\pi/2} \sin^4(\theta)\, \varphi\left(\frac{b\sin(\theta)}{\gamma l}\right) e^{-b^2\sin^2(\theta)}\, d\theta , \tag{14}$$

$$F_3(b) = \frac{\pi}{16}\left(\frac{E_\perp \gamma l}{E_p}\right)^2 e^{-b^2/2}\left[I_0\left(\frac{b^2}{2}\right) - I_1\left(\frac{b^2}{2}\right)\right] , \tag{15}$$

where $E_p = \gamma \Lambda \sqrt{2mT}/e\hbar$ and $I_n(y)$ is the modified Bessel function of order n.

III. RESULTS AND DISCUSSION

The dependence of the mobility on the temperature $\mu(T)$ is determined by the behavior of the denominator of the integrand of Eq. (12) for values of $x \leq 1$, since the main contribution to the integral comes from values of x in this range. So, the mobility depends on the behavior of the functions F_1, F_2 , and F_3 taken with the argument $k_T\, l$. For fields lower than $E_\perp = 500$ V/cm, the contributions coming from F_2 and F_3 are negligible and the overall temperature dependence of the mobility is entirely due to the function F_1. Unfortunately, this function cannot be given in an analytical form. However, it is possible to write expressions in the limit of very small and large arguments. For $b \ll 1$,

$$F_1(b) = \frac{5\pi}{32} b^2 \left[\ln^2\left(\frac{b}{\gamma l}\right) - 0.1274\, \ln\left(\frac{b}{\gamma l}\right) + 0.0158\right] , \tag{16}$$

and for $b \gg 1$

$$F_1(b) = \frac{\sqrt{\pi}}{4}\frac{(\gamma l)^4}{b^5} . \tag{17}$$

It is clear from the equations above that $F_1(b)$ decreases very fast as b goes to zero leading to an x^2 dependence of the denominator of the integral in Eq. (12). In order to avoid the divergence in the integrand as x tends to zero, we maintain F_2 and F_3 in the denominator, since they have a weaker dependence on x, because when b goes to zero, $F_2(b) \sim b$ and $F_3(b)$ tends to a constant value.

In Fig. 1 we show the function $F_1(b)$ for three values of l. As we can see, $F_1(b)$ has a maximum whose position, $b_{\max}$, shifts to the region of smaller b with decreasing l. However, this displacement is very small. Correspondingly, the accessible range of $b_T = k_T\, l$ where k_T is in the interval of interest ($1 < T < 10$ K) changes, with varying l, in a stronger way (see Table I). As l becomes larger, the range of the variation of b_T moves farther to the right from $b_{\max}$. As a consequence, at large enough values of l the maximum of $F_1(b)$, which leads to the minimum on $\mu(T)$, should be only observed at low enough temperatures, even for $T < 1$ K, as the consequence of the condition $b_{\max} < b_T$. With decreasing l the range of b_T tends to $b_{\max}$ and the minimum of $\mu(T)$ shifts to higher temperatures entering the interval of experimental interest $1 < T < 10$ K. By further decreasing l, the range of b_T tends to $b < b_{\max}$. At such a condition the minimum of $\mu(T)$ can be at $T > 10$ K, i.e., out of the

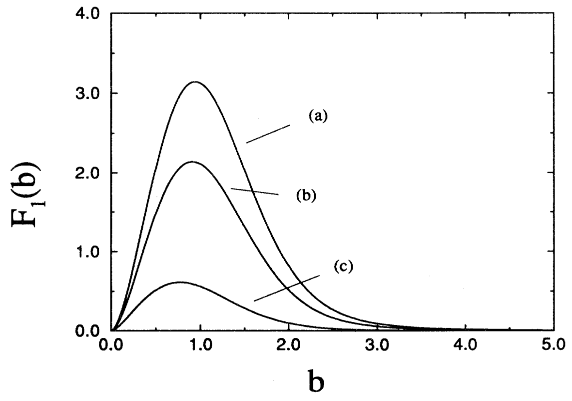

FIG. 1. The function $F_1(b)$ for three values of l : (a) 10^{-5} cm, (b) 5×10^{-6} cm, and (c) 10^{-6} cm.

TABLE I. Values of $b_{\max}$ and b_T in the temperature interval $1 < T < 10$ K.

l (cm)	$b_{\max}$	b_T
10^{-5}	0.94	4.7–15.0
5×10^{-6}	0.91	2.35–7.5
10^{-6}	0.77	0.47–1.5

temperature interval which is of our interest. So, when the minimum of $\mu(T)$ at large enough l is found at temperatures lower than 1 K, $\mu(T)$ increases monotonically in the interval $1 < T < 10$ K. At smaller l the minimum should be observed in this temperature range. For l so small that the minimum of $\mu(T)$ is found at $T > 10$ K, $\mu(T)$ is a decreasing function of temperature in the range $1 < T < 10$ K.

As can be noted from Eq. (12), the value of $T = T_{\min}$, which corresponds to the minimum of $\mu(T)$, depends on the behavior of the function $TF_1(k_T l)$. One can expect the minimum value when $TF_1(k_T l)$ begins to decrease more strongly than T^{-1}. Under such a condition $TF_1(k_T l)$ becomes a monotonically decreasing function of temperature and $\mu \sim [TF_1(k_T l)]^{-1}$ transforms into an increasing function of the temperature. For a better analysis it is convenient to introduce the temperature $\widetilde{T}$ in which $F_1(k_T l)$ has a maximum. The dependence of the mobility on the temperature is different in three regions: (i) For $T < \widetilde{T}$, $F_1(k_T l)$ is an increasing function of temperature. For this region $\mu \sim [TF_1(k_T l)]^{-1}$and decreases more strongly than $\mu \sim T^{-1}$. (ii) For $\widetilde{T} < T < T_{\min}$, $F_1(k_T l)$ decreases and $[TF_1(k_T l)]$ increases more slowly than linearly with T and the mobility decreases according to the law $\mu \sim T^{-a}$, where $a < 1$. (iii) For $T > T_{\min}$, $F_1(k_T l)$ decreases more strongly than the inverse of T, $[TF_1(k_T l)]$ decreases with increasing temperature, and the mobility is an increasing function of temperature.

The temperature ranges enumerated above depend strongly on l. The curve $F_1(k_T l)$ becomes a very smooth function at small values of l. For small enough l in a wide range of $k_T l$ around $b_{\max}$, $F_1(k_T l)$ can be treated as a constant. Under such a condition, the temperature dependence of mobility should behave like T^{-1}. If $T_{\min} > 10$ K, this behavior can take place at temperatures $T < 10$ K. However, with further decreasing l, $\widetilde{T}$ can be shifted to higher temperatures and, for values of $T < 10$ K, we can expect a stronger decrease of μ with the temperature than T^{-1} when $[TF_1(k_T l)]$ increases more strongly than T. In the experiments of Refs. 3 and 4, the temperature dependence $\mu \sim T^{-1}$ was observed at $5 < T < 12$ K. The usual electron-vapor scattering dominates the dependence of μ at higher temperatures. According to our analysis, the dependence $\mu \sim T^{-1}$ can be only obtained theoretically for a limited range of values of l . We obtain the best agreement with the results of Ref. 4, $\mu \simeq 8 \times 10^4/T$ cm^2/V s, for $l = 5 \times 10^{-7}$ cm and $\xi_0 = 2.58 \times 10^{-8}$ cm. In our calculation we put in Eq. (12), m equals the free electron mass in agreement with the results of Ref. 4 and the value of the holding field was taken as $E_\perp = 300$ V/cm. However, its influence on the results of the calculation is negligible.

In Fig. 2 the results of our calculation of $\mu(T)$ are presented (full line) with the experimental points taken from Ref. 4, where the dotted line is the best fit of the experimental values and the filled triangles correspond to the best hydrogen sample. For $T < 5$ K the experimental values of the mobility show a more weak temperature dependence than T^{-1}. This result cannot be explained if l and ξ_0 are constants: for given l and ξ_0, by lowering the temperature, $\mu(T)$ depends on T more strongly than T^{-1}. However, by decreasing the temperature from 12 K to 5 K, there occurs an essential deposition of hydrogen from the vapor to the surface which is negligible at lower temperatures and the quality of the surface improves.[4] According to this fact the model of ensemble average Gaussian correlation given by Eqs. (10) and (11) can be invalid at $T < 5$ K. The correct description of $\mu(T)$ in the whole temperature range requires a microscopic model of the surface itself which takes into account in some way an explicit dependence on temperature. However, the change of the surface profile at $T < 5$ K, due to the absence of the deposition of hydrogen atoms, can be qualitatively considered in the framework of the Gaussian fluctuation model. Indeed, under such conditions we may expect an increase in l and a decrease in ξ_0 as compared with their values when $T > 5$ K. In order to illustrate this behavior we calculated the mobility for a new set of values of these parameters. The results of the calculation at temperatures below 5 K depend strongly on the value of l, as shown in Fig. 3. However, we see in Fig. 2 that the results of μ for $l = 1.1 \times 10^{-6}$ cm and $\xi_0 = 2.07 \times 10^{-8}$ cm exhibit a theoretical dependence on the temperature which does not contradict the experimental data .

Finally, one can note that according to Ref. 4, $\mu(T)$

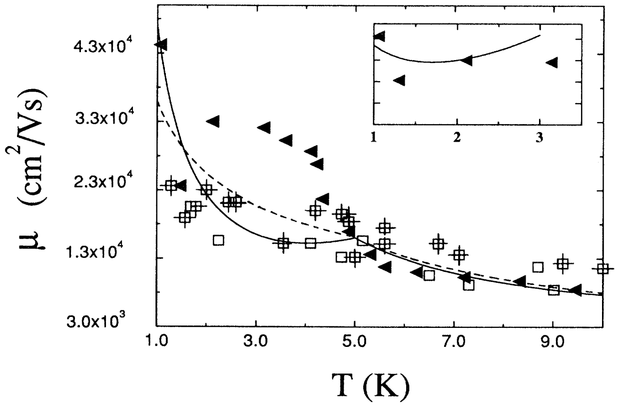

FIG. 2. The dependence of the electron mobility on the temperature. The theoretical curve (full line) corresponds to calculations using the following interface parameters: $l = 5 \times 10^{-7}$ cm and $\xi_0 = 2.58 \times 10^{-8}$ cm for the temperature interval $5 < T < 10$ K and $l = 1.1 \times 10^{-6}$ cm and $\xi_0 = 2.07 \times 10^{-8}$ cm for the temperature interval $1 < T < 5$ K. The dotted line is the best fit of experimental data taken from Ref. 4 and the filled triangles represent the mobility data for the best hydrogen sample. The inset shows the minimum in the calculated mobility around 1.5 K using the parameters $l = 1.7 \times 10^{-6}$ cm and $\xi_0 = 3.4 \times 10^{-8}$ cm.

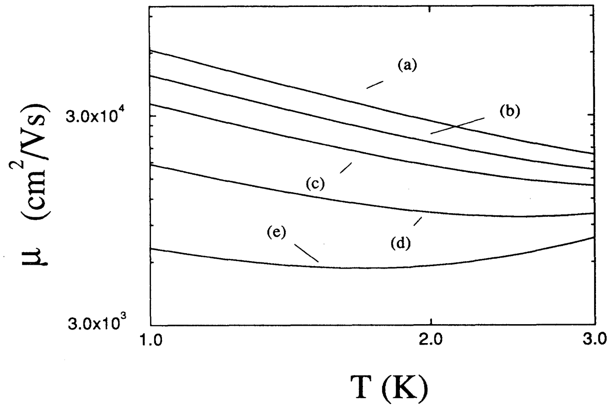

FIG. 3. The electron mobility as a function of temperature in the range $1 < T < 3$ K for different values of the interface roughness parameters: (a) $l = 10^{-6}$ cm and $\xi_0 = 2.0\times10^{-8}$ cm ; (b) $l = 1.1\times10^{-6}$ cm and $\xi_0 = 2.1\times10^{-8}$ cm; (c) $l = 1.2\times10^{-6}$ cm and $\xi_0 = 2.3\times10^{-8}$ cm; (d) $l = 1.4\times10^{-6}$ cm and $\xi_0 = 2.8\times10^{-8}$ cm; (e) $l = 1.7\times10^{-6}$ cm and $\xi_0 = 4.1\times10^{-8}$ cm. The values of ξ_0 were obtained by fitting the theoretical temperature dependences of the mobility with the experimental estimate $\mu = 8.0\times10^4/T$ cm^2/V s at $T = 5$ K.

obtained for the best hydrogen specimen shows a minimum near $T \approx 1.5$ K. We also tried to describe the nonmonotonic growth of $\mu(T)$ with the appearance of this minimum. Indeed, according to the theory developed in the present work, the well-pronounced minimum at $\mu(T)$ can be observed for a more or less ideal crystal with large enough l. We have obtained the minimum of $\mu(T)$ at $T = 1.7$ K for $l = 1.7\times10^{-6}$ cm and $\xi_0 = 3.39\times10^{-8}$ cm (see the inset of Fig. 2, where the calculated mobility is depicted along with the experimental points). However, in the interval $3 < T < 5$ K, the agreement of the theoretical curve and the experimental data obtained for the best specimen becomes worse probably due to the change of the surface structure at these temperatures.

IV. CONCLUSIONS

We have investigated theoretically the dependence of the mobility on the temperature of electrons localized over a solid hydrogen surface. We have employed the model of Gaussian correlations for the description of the surface roughness due to its simplicity (only two parameters l and ξ_0 are necessary which are defined as thermodynamically averaged lateral and vertical characteristics of defect sizes, respectively) and wide applications in other interfacial systems such as semiconductor heterostructures.[20–24] We have shown that the mobility of electrons is dominated by their scattering by the roughness of the hydrogen surface and the model used reproduces very well the experimental data in the temperature range $5 < T < 12$ K. An overall description of the surface indicates that the parameters obtained, ξ_0 (about 1–2 atomic sizes) and l (about 10^{-6} cm), agree well with the proposed model by Edel 'man and Faley,[4] in which the electrons are moving over flat terraces of size near 10^{-5} cm and scattered by defects with a height of about 1–2 atomic layers and a distance between defects of the order of 10^{-6}–10^{-7} cm. The values of ξ_0 also satisfy the condition $\xi_0 \ll \langle z\rangle_1$ that supports the validity of the perturbation theory[14] used to obtain the interaction potential given by Eq. (5). However, for temperatures $T < 5$ K, we found discrepancies between our results and the experimental data if we chose the same set of parameters as used in the previous range of temperature. Keeping in mind that the temperature dependence of the mobility is strongly dependent on the parameter l, we found different values of l and ξ_0 that give qualitatively the dependence of $\mu(T)$ and do not contradict the experimental fit. Furthermore, a minimum in the mobility, claimed by experimentalists,[4] is clearly shown in our calculation. We attributed the above-mentioned discrepancy to the absence of the deposition of hydrogen atoms from the vapor phase at lower temperatures, leading to smoother interfaces. However, other mechanisms have been proposed, such as a possible phase transition of the crystal structure or "the possibility that the solid hydrogen surface should be microscopically rugged on the atomic scale at temperatures near the triple point."[4] We believe that a theory of surface hydrogen growth, which is clearly beyond the calculation presented in this paper, and further experiments, are necessary to get a definite conclusion about the electron mobility in the low-temperature region ($T < 5$ K).

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