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Generalized picture of work function of a metal with Schottky interface

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Abstract

This paper discusses effects of metal on the Schottky barrier height. First, electron density effect on the Fermi level pinning at metal/Ge interface is considered, and then a metal work function in itself is reconsidered in conjunction with metal-induced gap states (MIGS) model. The metal work function depends on a counter material. This view may change how to understand the Schottky barrier formation mechanism

1. Introduction

Schottky barrier height (SBH) formation and Fermi-level pinning (FLP) mechanisms are fundamental in semiconductor devices, and have been discussed for a long time. Since SBH is determined by both the metal work function and electron affinity of a semiconductor in ideal Schottky limit, the work function in metal is one of key elements in SBH from the metal side. Although the work function in a metal is often regarded as a material constant, the contaminated surface exhibits unexpected values. This fact implies that the metal work function should be reconsidered in the Schottky interface by taking account of the contact with semiconductors. This paper discusses the FLP mechanism, and then reconsider the metal work function at the Schottky interface.

2. Work function and metal-induced gap states

The work function of a metal Φ_M consists of both the bulk and surface parts. The bulk part Φ_b comes from many electron effects, while the surface part Φ_s is from the wave function evanescent to the vacuum, which forms the surface dipole [1]. Although this view is too simple for quantitative discussion, the work function trend in many simple metals can be described on the basis of jellium model, as shown in **Fig. 1**. Since the surface part is in principle determined from the tunneling from the metal to vacuum, its penetration extent depends on the electron density and surface orientation of metals [2]. Note that the surface part in the work function looks similar to the physical implication of the metal-induced gaps states (MIGS) at metal/semiconductor interface originally proposed by Heine [3].

We have recently studied the effects of metal on FLP at metal/Ge interface from the aforementioned aspect. Namely, if the FLP on Ge may be predominantly characterized by the MIGS model, the FLP might be controlled by the electron density in metal and interface structure, as expected from the work function theory as shown in Fig.1 [4]. We prepared several kinds of germanides on n-Ge and measured their SBHs at room temperature. Although we do not presently know the exact work functions of germanides, the germanide

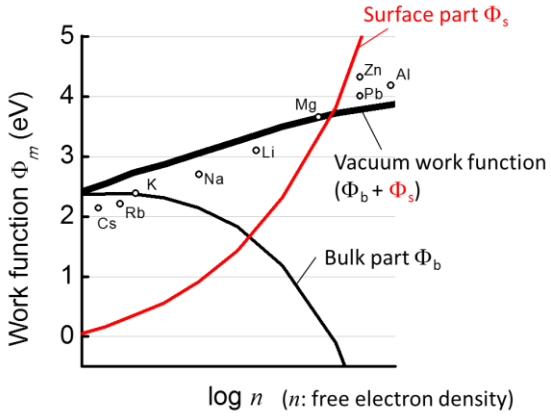

Fig. 1 Calculated bulk and surface terms of the vacuum work function as a function of free electron density in metal (Replotted from ref. 1). Note that Φ_s becomes dominant with free electron density increase.

with a rather low work function metal, $GdGe_x$, shows the higher I_{off} current on n-Ge (100). This implies the lower SBH at the $GdGe_x$ interface. More interestingly, $GdGe_x$ on n-Ge (111) exhibits ohmic I-V characteristics, as shown in **Fig. 2**, while a Gd/Ge junction does not show appreciable surface orientation dependence. It was also confirmed that no interface layer was formed at the $GdGe_x$/Ge interface by cross-sectional TEM. The electron density in $GdGe_x$ estimated by the Hall effect measurement was ~7 x10^{21} cm^{-3}, which is ~one order of magnitude lower than that in conventional metals. Although the present result is not necessarily conclusive for the SBH formation mechanism on Ge, it is strongly suggested that the free electron density in metals has a significant effect on the SBH formation in Ge. The experiments are still preliminary but the results are exciting.

Most of metal/Ge junctions without strong FLP trend reported so far [5–11] seem to be consistent with this view. We do not think a single mechanism always determines the FLP for a given semiconductor, including Ge, but a couple of mechanisms might work together. We think that the MIGS dominant behavior in Ge comes from the fact that Ge is a special semiconductor with a narrow energy band gap and less defects.

3. Reconsideration of work function

The work function Φ_M used in Eq. (1), in which Φ_M is the metal work function with the vacuum interface. As discussed in the previous section, the work function should be sensitive to the surface counterpart. Namely, the work function

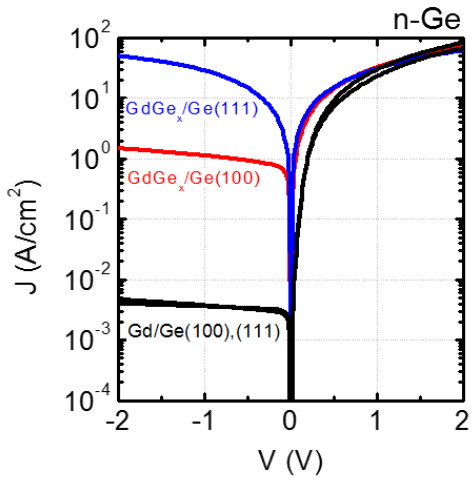

Fig. 2 Typical J-V characteristics of germanide and element metal/n-Ge(100) and /Ge(111) junctions. Note that $GdGe_x$/n-Ge(111) shows ohmic characteristics.

depends on what the counter interface is. Now, we come to the question "Is the work function at the Schottky interface Φ_M ?" In fact, Φ_M is very sensitive to the surface orientation and contamination. Therefore, we rewrite the metal work function in contact with semiconductors as follows, by assuming that any finite shift from the Schottky limit may come from the work function modulation on semiconductors.

$$\Phi_B = S(\Phi_M^V - \Phi_{CNL}) + (\Phi_{CNL} - \chi) = \Phi_M^{Semi} - \chi, \quad (1)$$

where $\Phi_M{}^V$ and $\Phi_M{}^{semi}$ are the work functions in vacuum and on semiconductor, respectively. And, Φ_{CNL} is the charge neutrality level from the vacuum level in the semiconductor side. That is,

$$\Phi_M^{Semi} = S\Phi_M^V + (1 - S)\Phi_{CNL}, \quad (2)$$

This equation means that $\Phi_M{}^{semi}$ is determined by both Φ_M and Φ_{CNL} with the weight of S and (1 - S). In case of S = 1, $\Phi_M{}^V = \Phi_M{}^{semi}$, while generally $\Phi_M{}^{semi}$ should be affected by the intrinsic wave function evanescent from metal to semiconductor, which is considered as the MIGS origin, resulting in the interface dipole formation at metal/semiconductor interface. This is the intrinsic effect affecting the work function on semiconductors (insulators as well) in the pure limit. The interface has been generally considered as ($\Phi_M{}^V$ + FLP), but note that $\Phi_M{}^V$ loses the physical meaning in a metal contacting with semiconductor. Thus, we would suggest that instead of such conventional view, the MIGS-type FLP can be regarded as the metal work function modulation ($\Phi_M{}^{semi}$ instead of $\Phi_M{}^V$ + FLP) in the Schottky limit, although the MIGS view is important in terms of the fact that $\Phi_M{}^{semi}$ is affected by the CNL in the semiconductor.

The present view does not necessarily exclude extrinsic origins such as defect effects. Equation (2) can be rewritten as

$$\Phi_M^{Semi} = S^M\Phi_M^V + (1 - S^M)\Phi_{CNL}^{MIGS}, \quad (2')$$

Suppose that there is an extrinsic FLP origin at the interface, with S^D and $\Phi_{CNL}{}^D$. In that case, SBH is described by Eq. (1) with $\Phi_M{}^{semi}$.

$$\begin{aligned}\Phi_B &= S^D\left(\Phi_M^{Semi} - \Phi_{CNL}^D\right) + (\Phi_{CNL}^D - \chi) \\ &= S^DS^M\left(\Phi_M^V - \frac{1}{1-S^DS^M}\left((1-S^M)S^D\Phi_{CNL}^{MIGS} + (1-S^D)\Phi_{CNL}^D\right)\right) \\ &\quad + \frac{1}{1-S^DS^M}\left((1-S^M)S^D\Phi_{CNL}^{MIGS} + (1-S^D)\Phi_{CNL}^D\right) - \chi, \quad (3)\end{aligned}$$

By newly denoting S and Φ_{CNL} in the following,

$$\begin{cases} S = S^DS^M \\ \Phi_{CNL} = \frac{1}{1-S^DS^M}\left((1-S^M)S^D\Phi_{CNL}^{MIGS} + (1-S^D)\Phi_{CNL}^D\right), \end{cases} \quad (4)$$

Eq. (1) is obtained again. It is noted here that two independent pinning mechanisms are involved in this formula, although an interaction between two origins is not considered. In case that $S^M \sim 0 << S^D$,

$$\begin{cases} \Phi_B = (S^D\Phi_{CNL}^{MIGS} + (1-S^D)\Phi_{CNL}^D) - \chi \\ S \sim 0 \\ \Phi_{CNL} = (S^D\Phi_{CNL}^{MIGS} + (1-S^D)\Phi_{CNL}^D), \end{cases} \quad (5)$$

Thus, it is expected that Φ_B has nothing to do with $\Phi_M{}^V$, and that Φ_{CNL} is also affected by the extrinsic FLP origin. It may correspond to the Ge case. When the metal side effect for the FLP is physically considered as discussed above, the relationship between SBH and metal work function will become physically clearer.

4. Conclusion

When the metal side effect for the FLP is physically considered. We have studied the SBH formation mechanism by reconsidering the work function of metal in contact with a semiconductor from the viewpoint of tuning the wave function evanescent. In case of strongly pinned semiconductors such as Ge, the present view is very important and useful for analyzing the Fermi-level pinning alleviation.

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