



# Proposal of a new physical model for Ohmic contacts

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## ARTICLE INFO

### Article history:

Received 31 August 2009

Received in revised form

13 January 2010

Accepted 3 February 2010

Available online 12 February 2010

### Keywords:

Ohmic contacts

Two-dimensional electron system

## ABSTRACT

Ohmic contacts are crucial for both device applications and the study of fundamental physics. In this study, we propose a new physical model for Ohmic contacts based on the detailed considerations of a metal/semiconductor interface, such as charge neutrality level concept, with which it is possible to describe the real situation precisely. Our proposed model contains many defect energy levels that originate from vacancies and impurities located in the vicinity of the metal/semiconductor interface, within the energy range of the Schottky barrier height. Moreover, we calculate the current–voltage characteristics based on our model. Our calculated results show that our model reveals linear Ohmic  $I$ – $V$  characteristics and dense defect energy level distribution in the energy range of the Schottky barrier height is crucial for obtaining Ohmic  $I$ – $V$  characteristics.

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## 1. Introduction

Low resistive Ohmic contacts are crucial for both device applications and the study of fundamental physics. To date, Au/Ge/Ni alloyed Ohmic contacts to two-dimensional electron gas embedded in AlGaAs/GaAs heterostructures have been reported [1,2]. In accordance with the requirement of anticipated device scaling, nano-scale Ohmic contacts are expected in the future [3]. Moreover, in order to introduce the metal source/drain electrodes that will be required for transistors in the future, it is essential to establish a technology to fabricate Ohmic contacts between these electrodes and the substrate materials.

An Ohmic contact is defined as metal/semiconductor contact that has negligibly lower contact resistance than the bulk resistance [4]. In contrast, a Schottky barrier is a potential barrier that is formed at a metal/semiconductor interface, as shown schematically in Fig. 1(a), and which causes rectifying properties. In general, Ohmic contacts can be understood by reference to two band diagrams [4]. One features a reduction in the thickness of the Schottky barrier shown schematically in Fig. 1(b). This is achieved by increasing the doping density. The other involves a lowering of the Schottky barrier height, as shown schematically in Fig. 1(c). For future devices, it is anticipated that the precise control of the Schottky barrier height will play an important role. However, we consider that conventional fabrication processes are not suitable for nano-scale Ohmic contacts because of the difficulties that are introduced by nano-scale control.

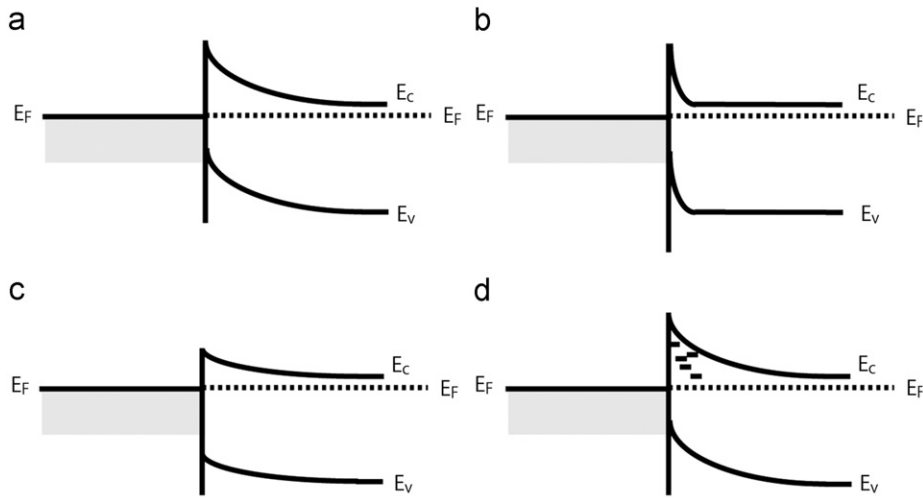
Identically, according to the theory of interface physics, it is known that the Fermi levels of metals are pinned to the charge neutrality level of the semiconductor when metal surfaces are in contact with semiconductor surfaces (metal/semiconductor interfaces are formed) [5,6]. Moreover, it has been reported that the pinning positions are almost independent of the metal species, since the density of the interface states is remarkably high [5].

Accordingly, it is indicated that the conventional band diagrams for Ohmic contacts are contradictory to our knowledge of interface physics, i.e. Fermi level pinning phenomena. According to these phenomena, reducing Schottky barrier height is very difficult in ‘real’ situation. In other words, the conventional model significantly disagrees with the observation for fabricated Ohmic contacts. In this study, we propose a new physical model for Ohmic contacts based on the detailed considerations of a metal/semiconductor interface, such as the charge neutrality level concept, with which it is possible to describe the real situation precisely. Furthermore, it is crucial to understand Ohmic contacts in correct band diagrams for future nano-scale contact fabrication. Moreover, we calculate the current–voltage ( $I$ – $V$ ) characteristics varying the energy distribution of the discrete levels within the Landauer scheme.

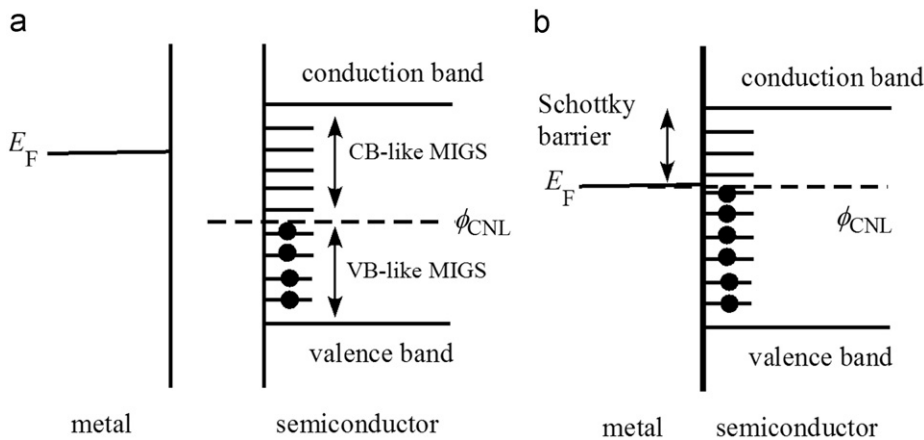
## 2. Fermi level pinning and charge neutrality levels

In the 1980s, a number of works were reported related to the Schottky barrier heights of metal/semiconductor interfaces. Among these reports, the concept of the ‘charge neutrality level’ is quite efficient for predicting and analyzing Schottky barrier heights [5,6].

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**Fig. 1.** Schematic illustrations of the metal/semiconductor contact. (a) Schottky barrier. (b) Ohmic contact achieved by reducing the thickness of the Schottky barrier. (c) Ohmic contact achieved by lowering the Schottky barrier height. (d) Our proposed model for Ohmic contact.



**Fig. 2.** Schematic band alignment at metal/semiconductor interface (a) before and (b) after contacting. The Fermi energy of the metal tends to move toward the charge neutrality level,  $\phi_{CNL}$ , by transferring electrons around the interface (bold lines).

At the metal/semiconductor interface, in general, the semiconductor possesses electronic eigenstates that have eigenenergies within the band-gap of bulk semiconductor. These states appear because the translational symmetry of semiconductor bulk crystals is broken at interfaces perpendicular to the interface direction, and thus the phenomenon that produces the band-gap in the energy spectrum and which forbids the existence of eigenstates within the band-gap disappears. These states consist of eigenstates in the complex band structures of the bulk materials and have complex wave numbers; thus, they are localized around the interface and are known as ‘evanescent-wave states’. Such states are also called ‘metal-induced gap states’ (MIGS) and are shown schematically in the energy diagram in Fig. 2(a). Actually, Louie and Cohen [7] demonstrated by *ab initio* calculations of the electronic structures of Al/Si interfaces that these states really exist in semiconductors around the metal/semiconductor interfaces.

As shown in Fig. 2(a), some of the MIGS are occupied from the bottom corresponding to the number of electrons around the interface, and the highest occupied MIGS determines the effective Fermi energy of the semiconductor around the interface. Since this Fermi energy is determined by the electron number to maintain the semiconductor as neutral, it is called the ‘charge neutrality level’ ( $\phi_{CNL}$ ). When the semiconductor forms a contact with a metal, as shown in Fig. 2(b), electrons in the semiconductor

and the metal move across the interface to equalize their Fermi energies,  $\phi_{CNL}$  and  $E_F$ , which results in the final band alignment at the interface. This means that the Schottky barrier heights are insensitive to the metal species. This phenomenon is called ‘Fermi-level pinning’, and gives good agreement with the reported experiments [5,6].

### 3. Model and method

#### 3.1. Model

As discussed in the previous section, it is very difficult to control the Schottky barrier heights at metal/semiconductor interfaces by changing the metal species due to Fermi-level pinning. This means that it is difficult to design metal/semiconductor interfaces that have band diagrams that are characteristic of Ohmic contacts, shown in Fig. 1(c). However, such Ohmic contacts (linear  $I$ - $V$  characteristics) have actually been observed experimentally [1]. These considerations lead to the necessity of identifying a new model for Ohmic contacts.

In this study, we propose a new model for the Ohmic contacts with the band diagram described in Fig. 1(d). It contains many discrete energy levels that originate from defects located in the

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