DEEP LEVELS AND BAND BENDING AT METAL-SEMICONDUCTOR INTERFACES

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Introduction

Over the past several decades, a common theme of metal-semiconductor interface studies has been the insensitivity of semiconductor band bending to the properties of different metal overlayers and the physical mechanisms responsible for this Fermi level "pinning". Hampering efforts to identify the nature of charge transfer at these electronic junctions has been the narrow ranges of reported Fermi stabilization energies themselves, which permit a number of quite dissimilar explanations. Furthermore, evidence for charge states at metal-semiconductor junctions has been indirect for the most part, relying heavily on electrostatic measurements. Experimental and theoretical work over the last few years has contributed new information which challenges the commonly accepted view of semiconductor contact rectification. First of all, experimental evidence now exists to show that semiconductors, even those previously thought to be strongly "pinned", exhibit wide ranges of Fermi level stabilization with different metal overlayers. Secondly, it is now possible to observe interface states directly by optical techniques and to demonstrate their direct relationship to Fermi level stabilization at the microscopic electronic junction. Furthermore, these states confirm the predictions of a microscopic electrostatic model for the detailed band bending measurements over wide energy ranges. Recent developments have also highlighted the importance of surface processing and bulk crystal quality in terms of the deep levels formed and their subsequent role in rectification at less than-ideal interfaces. In
contrast, experiments performed at low temperature on high quality interfaces permit a closer approach to ideal chemical junctions and a striking contrast with more conventional measurements of the same systems. Given the much wider array of band bending and deep level information now available, it is now possible to draw sharp distinctions between many of the various models which have been advanced to describe the charge transfer between metals and semiconductors. What emerges is a picture similar to that advanced fifty years ago by Schottky in terms of macroscopic electrostatic parameters, but complicated by the formation of chemically-induced native defects and interfacial phases.

**Band Bending and Interface States: Historical**

Two basic elements of contact rectification at metal-semiconductor interfaces are 1) the physical nature of the electronic states at the interface and 2) the relative magnitudes of the interface and surface space charge dipoles which together comprise the potential difference between the initial interface components. Dipoles form at free semiconductor and metal surfaces due to the charge distributions which extend into vacuum. A new dipole forms at the metal-semiconductor junction which can involve tunneling as well as discrete localized charge states. The latter can be due to: changes in semiconductor lattice bonding, adsorbate-semiconductor bonding, surface defects, bulk defects segregated to the surface, native defects induced by a metal-semiconductor reaction or diffusion, impurities, extended lattice imperfections, as well as new interface chemical phases. There is now extensive evidence to show that metals and semiconductors can interact strongly, thereby giving rise to one or more of these extrinsic interface state phenomena.

The charge in the interface states will determine the magnitude of the interface dipole and thereby the portion of the junction electrostatic potential difference which falls across the semiconductor’s band bending region. For tunneling states, the magnitude of the dipoles and their change upon junction formation can be determined via a variety of microscopic model calculations. However, the results depend sensitively upon the detailed boundary conditions chosen, which can produce completely disparate conclusions. For example, the boundary condition of a relatively constant barrier height itself necessitates a large interface dipole for tunneling calculations involving a charge neutrality level. Calculations which model the metal electronic density as “jellium” and impose bulk lattice properties at the interface also obtain large interface dipoles which dominate the charge transfer. Here the total voltage change is required to occur completely at the microscopic junction. In contrast, a