Comment on "Electronic Structure of Ideal Metal/GaAs Contacts"

In an interesting paper [1], van Schilfgaarde and Newman have analyzed theoretically the electronic structure of ideal metal/GaAs contacts by means of a self-consistent local-density approximation (LDA), and have concluded that "models which invoke intrinsic interface states to explain Fermi-level pinning are not consistent with experimental observations. This strongly suggests the nonideal nature of the experimentally observed interfaces."

Contrary to these remarks, I intend to show that ideal interfaces and the induced-density-of-interface-states (IDIS) model (or the intrinsic-interface-states model in Ref. [1]) can explain the observed behavior of metal-semiconductor interfaces.

The conclusions of Ref. [1] are based on the theoretical results obtained for the barrier heights of different metal/GaAs interfaces that show a lack of correlation with the experimental evidence and, apparently, with the charge-neutrality level of the IDIS model [2]. Leaving apart the problems associated with the error introduced [3] in the LDA, which makes the conclusions of Ref. [1] at least questionable, I would like to concentrate on the actual characteristics of the IDIS model. First of all, I should mention that it has already been known for some years that the IDIS model would yield different interface change-neutrality levels depending on the interface conditions [4,5]. Accordingly, intrinsic and extrinsic charge-neutrality levels have been introduced [6]. The intrinsic level (or the midgap energy [2]) only appears in very idealized conditions: (i) where the metal has a broad and featureless electronic density of states [7]; and (ii) for (110) III-V semiconductor surfaces, when the adsorbed metal atom is very large, and its valence electrons interact similarly with the cationlike and the anionlike surface states [7,8].

Even Al on Si(111) can give [4] different charge-neutrality levels depending on the position of the last Al layer on the Si surface. Theoretical results yield values of ϕ_{Bp} ranging between 0.4 and 0.9 eV, depending on the surface geometry. These values fluctuate around 0.67 eV, the level that one can define as the Si intrinsic charge-neutrality level [6].

K on GaAs(110) is a very ideal case [8] due to the K large size. The charge-neutrality level and the Fermi energy are almost independent of the metal adsorption site, yielding a Schottky barrier ϕ_{Bp} of $\sim$0.7 eV.

For a thick Ag-GaAs(110) interface it has been found [5] that the Schottky barrier ϕ_{Bp} varies between 0.54 and 0.93 eV, depending on the metal adsorption sites on the semiconductor. The intrinsic charge-neutrality level was also found [5] to be around 0.7 eV.

The important point that one can deduce from these results [2–4] is *that the extrinsic charge-neutrality level fluctuates around the intrinsic one,* depending on the metal-atom properties (as shown very elegantly in Ref. [1]) and its adsorption site at the semiconductor interface.

The results of Ref. [1] seem to confirm this conclusion, since the calculated values of ϕ_{Bp} fluctuate around 0.7 eV, the GaAs intrinsic charge-neutrality level [6]. On the other hand, those results have been calculated for a fixed interface geometry: One can expect, however, for the metal adatoms different adsorption sites from the ones assumed in Ref. [1], changing accordingly the interface Fermi level.

In conclusion, the actual theoretical evidence [4–6] does not support the claim of Ref. [1] mentioned at the beginning of this Comment and suggests that more theoretical calculations minimizing the total interface energy are necessary before a definitive conclusion about the properties of ideal metal/GaAs contacts can be reached. Let us remark, however, that LCAO calculations along these lines have been performed for the alkali-metal–GaAs(110) interfaces [8,9]; the results of these calculations support unambiguously the IDIS model. Moreover, LDA calculations [3] for the $NiSi_2$-Si junction for which the interface geometry is well established also support the same model. All these results suggest the ideal nature of at least some of the experimentally observed interfaces.

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F. Flores
Departamento de Fisica de la Materia Condensada
Universidad Autónoma
28049 Madrid, Spain

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