# Summary Abstract: The effect of doping on Fermi level position at a semiconductor–metal interface[a)]

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Recent experiments, involving thin coverage of metal atoms on III-V semiconductors, suggest that the Fermi level position at the surface for *n*- and *p*-type materials may differ by as much as 0.2 eV.[1] However, in measurements of Schottky barriers consisting of a bulk metal against a bulk semiconductor, the Fermi level position at the metal–semiconductor interface is found to be the same for both *n*- and *p*-type semiconductors to within 0.1 eV.[2]

To understand this difference, we have investigated the phenomenon of Fermi level pinning by charged interface states at the semicondutor–metal interface. Two limiting cases were investigated. In the first case, we modeled an interface with an infinitely thick metal. In the second case, we modeled a submonolayer coverage by using a free semiconductor surface containing defects. In both cases, we assumed that most of the defect induced interface states are localized a few angstroms inside the semiconductor. Under these conditions we have estimated the difference in Fermi level position between *n*- and *p*-type semiconductors to be less than 0.05 eV in the case of a thick metallic coverage, which agrees with the theoretical results of Daw and Smith.[3] This difference was shown to be the maximum one, and it occurs only when there is no pinning by the defects. When there is pinning, this difference is even smaller. No such upper bound on the difference in Fermi level position exists in the case of submonolayer coverage. We have also found that the number of interface states required to pin the Fermi level is $\approx 10^{14}$ cm$^{-2}$ in the case of coverage by a thick metal, but only $\approx 10^{12}$ cm$^{-2}$ in the case of a submonolayer coverage.

In the case of a submonolayer coverage, our results agree with the experimental results for thin coverage reported by Spicer *et al.*[1] and others. Our calculations for thick metallic coverage, however, differ qualitatively from those obtained in the submonolayer limit. This difference between thin and thick coverage is due to the fact that there are actually two very distinct pinning mechanisms at work in the two cases. The difference in the two mechanisms results from the difference in the main source of charge that balances the charge on the interface states. With $10^{12}$–$10^{13}$ states/cm$^2$ but without substantial metal coverage, these charges come from shallow impurities in the semiconductor bulk. The requirement of total charge neutrality will determine the Fermi level position, and the Fermi level position can differ substantially between *n*- and *p*-type semiconductors.[4] For the case of a bulk metal, the charge in the interface layer is balanced mainly by charge in the metal, setting up a very thin dipole layer. The charge in the metal can easily respond in such a way as to balance the depletion charge, and hence, the *n*- and *p*-type pinning positions are very similar.

In Fig. 1 we show our model for the macroscopic Schottky barrier. It consists of an abrupt interface between a semi-infinite metal and semiconductor. A sheet of charged defects, a few angstroms inside the semiconductor, forms a dipole layer with charges in the metal.[5] This dipole layer can be viewed as a charged parallel plate capacitor. The voltage in this layer can account for part of the difference between the semiconductor electron affinity and the metal work function. The rest of this difference is accommodated in the depletion region inside the semiconductor and in some potential difference inside the metal near the interface.[6]

In Fig. 2 we show the position of the Fermi level at the interface for the case of bulk metal coverage on both *n*- and *p*-type semiconductors. The semiconductor parameters were taken to be those of GaAs with doping concentration of $10^{17}$ cm$^{-3}$. The energies of the interface states correspond to those suggested by Spicer *et al.*[1] for GaAs, and we assumed that they all lie 5 Å from the metal surface. The density of interface donors and acceptors was assumed to be $10^{14}$ cm$^{-2}$ each. We assumed that both interface donors and acceptors were present. A similar calculation with an interface state density of $10^{13}$ cm$^{-2}$ did not show any substantial pinning. One can see that the difference in Fermi level position between *n*- and *p*-type is always less than 0.05 eV and that this difference occurs only when there is no pinning. One can also see that for a given metal work function, either the inter-

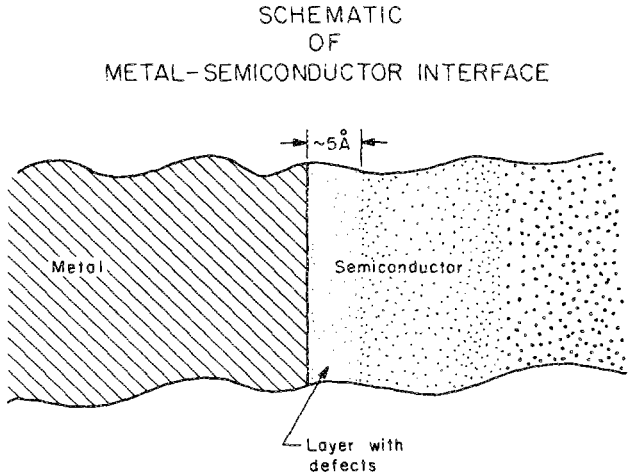


FIG. 1. Geometry of the metal semiconductor interface, including charged interface states.

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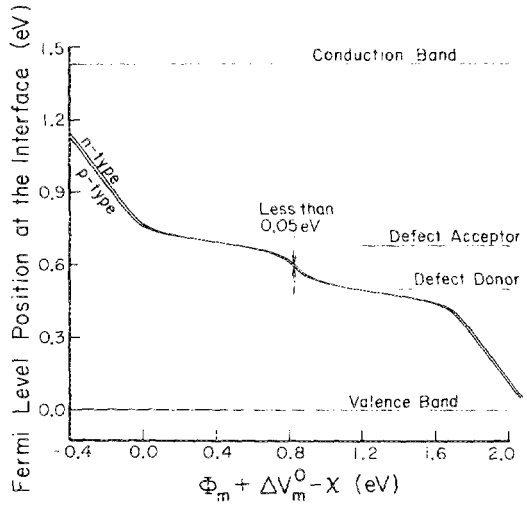


FIG. 2. Position of the Fermi level at the interface vs metal work function ($\Phi_m$) for the case of bulk metallic coverage on $n$- and $p$-type semiconductors. $\chi$ is the electron affinity of the semiconductor, and $\Delta V_0$ is the potential difference between the metal surface and bulk.

face acceptors or the interface donors (but not both) are being charged, resulting in two pinning levels for different work functions but independent of the semiconductor doping.

In Fig. 3 we show the Fermi level position at the surface versus the defect induced interface state concentration for our submonolayer coverage model. We assume that all the charge for the interface states has come from the semiconductor. One can see that when the interface states concentration reaches $10^{12}$ cm$^{-2}$, the Fermi level position is almost stabilized. (When the density of interface states increases further, the $n$- and $p$-type lines will asymptotically approach each other due to partial compensation,[7] but this effect is hardly noticeable on this scale.) The position of the Fermi level is independent of the type of the adatom if we assume that the only role the adatom plays is to induce native defects in the semiconductor. One can also see that the position of the Fermi level may be significantly different between $n$- and $p$-type semiconductors at that concentration of interface states.

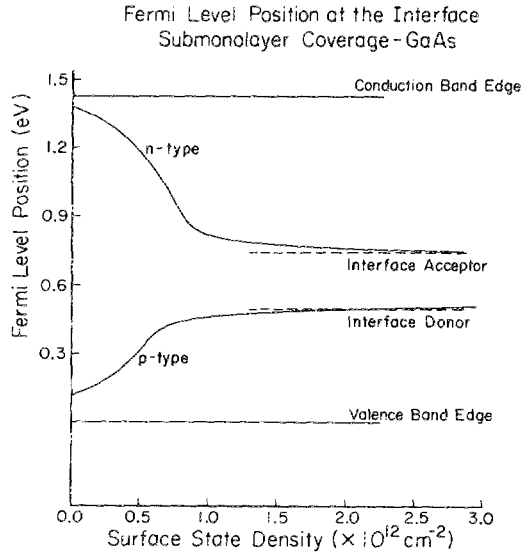


FIG. 3. The position of the Fermi level at the interface vs density of surface donors (and acceptors) for the case of submonolayer coverage on $n$- and $p$-type semiconductors. We assume arbitrarily that there are an equal number of donor and acceptor states.

The detailed analysis of this model, modifications for more than one type of interface state, defects with three charge states, and different spatial arrangement of the interface states as well as analysis of the metal response for excess charge will appear in a forthcoming paper.[6]

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[1] See, for example, W. E. Spicer, I. Lindau, P. Skeath, and C. Y. Su, J. Vac. Sci. Technol. 17, 1019 (1980).
[2] C. A. Mead, Solid State Electron. 9, 1023 (1966).
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[6] A. Zur, T. C. McGill, D. L. Smith, Phys. Rev. B (to be published).
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