Schottky-Barrier Formation and Metallicity

Two recent Letters[1,2] suggested a correlation between the occurrence of changes in the Fermi-level position and the clear occurrence of metallic behavior in the deposited metal. The key question is that of unambiguous criterion for the occurrence of metallic character. We question the criteria used in the cited papers and propose different criteria.

The bulk metal Fermi cutoff measured in photoemission spectroscopy is given by a characteristic line shape (step function convoluted with the instrument broadening) that is bisected by the Fermi level, giving a clear criterion for metallization. This is illustrated in Fig. 1 showing the Fermi cutoff and Fermi level of bulk Ag and Pd (from Wertheim, DiCenzo, and Buchanan[3]). Also included in the figure are curves from the Tm/GaAs Letter of Prietsch *et al.*[1] In that Letter a sharp change in the GaAs surface Fermi-level position between Tm coverages of 2.0 and 2.8 Å of Tm was correlated with the appearance of metallicity in the Tm film as judged by the curves in the figure. Their criterion is the Fermi level moving into the leading edge of the cutoff; however, there seems to be no justification for this, especially when no correction is made for instrumental broadening (0.15 eV here).[1] In fact, we find no clear evidence of metallicity for largest coverages used (7.2 Å). In earlier work with rare-earth metals (Tb, Dy, and Er) on GaAs, Waldrop[4] found that substantial interface chemistry occurred with the formation of a nonmetallic arsenide interfacial layer greater than 12 Å thick separating the GaAs and the rare-earth metal films. Since Prietsch *et al.*[1] show that their Tm deposits are similarly highly reactive, it seems reasonable to suggest that it may not be metallicity but complex chemistry which produces the change in Fermi level.

In the work by Stiles and Kahn,[2] experimental difficulties prevented determination of the Fermi cutoff. The criterion for the occurrence of metallicity is based on an increase in width of the Ag-4*d* states due to band-structure effects. These authors related their work to that of Wertheim, DiCenzo, and Buchanan[3] who, however, did not equate development of the width of the Ag-4*d* states with metallicity. In fact, there seems to be no clear relationship between the 4*d* width and the occurrence of metallicity. Zur, McGill, and Smith[5] argue that, when a metal is in contact with a semiconductor, the Fermi levels for *n*- and *p*-type materials must coincide; however, in Ref. 2 this is not seen. Thus, by the criterion of Zur, McGill, and Smith one can argue that the Ag film never achieves metallicity.

It is not the purpose of these comments to argue against the metal-induced gap states as a viable mechanism for the Fermi-level pinning, but rather to question whether the criteria given for metallicity in the cited papers are unambiguous. In addition, we argue for the development of definitive criteria for the of metallicity being clearly established in thin films. More work is also needed to relate these criteria to those necessary for the metal-induced gap state mechanisms to become operative.

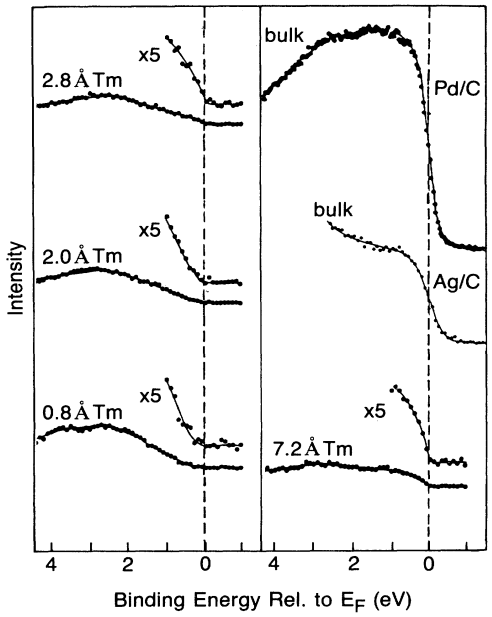

FIG. 1. Left-hand panel: photoemission spectroscopy spectra for various coverages of Tm/GaAs (Ref. 1). Right-hand panel: photoemission spectroscopy spectra for 7.2 Å Tm on GaAs and for bulk Ag and Pd (Ref. 3).

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