

SURFACE STATES ON SEMICONDUCTOR CRYSTALS; BARRIERS ON THE Cd(Se:S) SYSTEM

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SURFACE STATES ON SEMICONDUCTOR CRYSTALS; BARRIERS ON THE Cd(Se:S) SYSTEM

(composition effects; Fermi level; work function; E)

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We report here measurements of surface barrier heights of metal contacts on Cd(Se:S) crystals in which a continuous transition is observed between the CdS case in which the barrier height varies as the metal work function to the CdSe case where the barrier height is essentially independent of the metal. The results have fundamental implications concerning the nature of the surface states and their relationship to the properties of the semiconductor.

It was first pointed out by Shockley¹ that surface states on semiconductors fall into two distinct classes, depending on the nature of the semiconductor. For the more ionic materials, with small overlap between adjacent atoms, surface states should occur just above the valence-band edge and just below the conduction-band edge. For the more covalent materials with large overlap, the surface states should occur in a narrow half-filled band near the center of the forbidden gap. In the former case, surface barriers made by placing a metal in intimate contact with the surface should show a barrier height roughly proportional to the work function of the metal. In the latter case the height of the barrier should be nearly independent of the metal used.² Thus the measurement of barrier heights is a convenient method to evaluate the nature of the surface states on any given semiconductor. Both types of behavior have been observed experimentally,³⁻⁶ but since a continuous transition between the two has not been observed previously it has been difficult to correlate nature of the surface states with the bulk properties of the semiconductor.

Barriers used in the present study were prepared by cleaving small crystal samples in a vacuum and immediately evaporating a metal layer on the cleaved surface. Barrier heights were measured by the photoresponse technique, together with the voltage variation of the capacitance and the forward characteristic. The entire procedure has been described in detail previously.³ Composition of the crystals was determined by x-ray fluorescence. Barrier heights obtained for several metals are shown as a function of semiconductor composition in Fig. 1. The barrier heights on the CdS vary widely with the metal used, approximately as the metal work func-

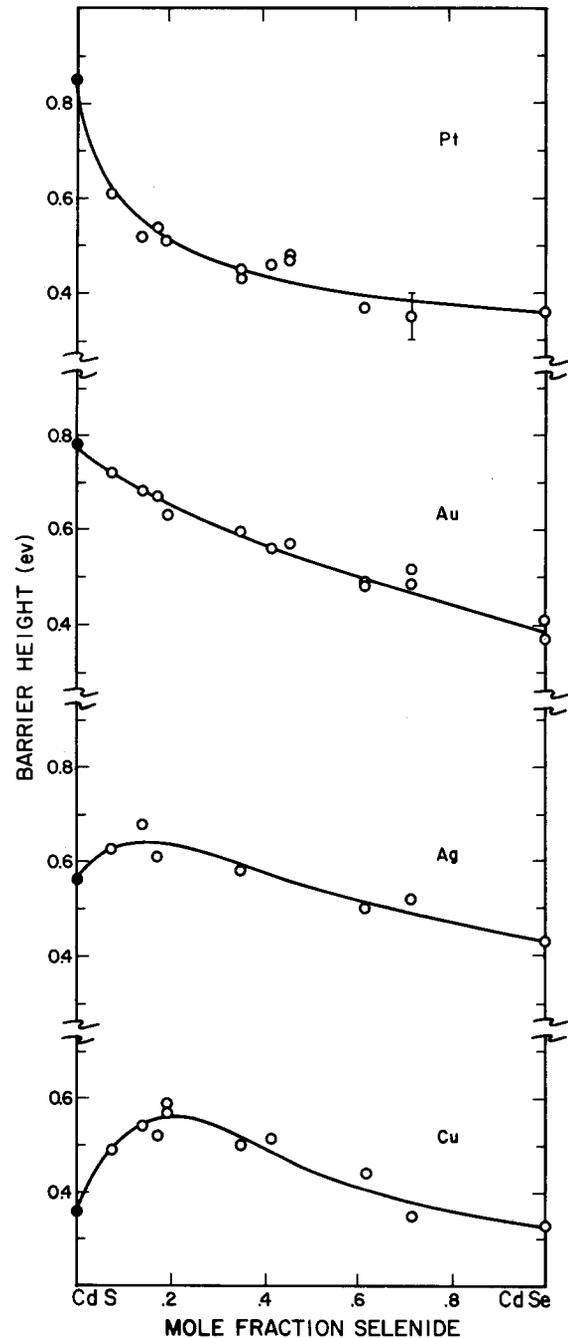


Fig. 1. Barrier heights of metals on Cd(Se:S) crystals as a function of crystal composition; ordered as to metal work function. CdS points taken from ref. 3.

tion, as noted previously.³ In this case the surface states are close to the band edges, and the Fermi level at the interface can move up or down in energy over a relatively large range without requiring any surface charge to fill or empty these states. On the CdSe end, however, the surface states lie in a narrow band in the forbidden gap, and the Fermi level at the interface cannot move appreciably without filling or emptying a large number of surface states and hence is "pinned" at a given energy.⁸ As the crystal composition is made richer in selenium, the overlap between adjacent atoms is increased, the surface states move toward the center of the gap, the Fermi level at the surface is "squeezed" between them, and a continuous transition is observed between the work-function-controlled case and the surface-state-controlled case. We believe that these results represent a striking verification of the role of surface states in the metal-semiconductor barrier and shed light on the fundamental relationship between the nature of surface states and the bulk properties of the semiconductor. It is hoped that these results will stimulate further theoretical work on surface states and the nature of metal-semiconductor contact.

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⁸It will be noted that the curves for the various metals do not exactly superimpose at high selenium concentrations. This is presumably due to a small perturbation of the surface state by the metal which is obviously not related to the work function. Of course if enough charge is supplied to completely fill the surface states (as, for example, by a very electropositive metal), barrier can be reduced or even destroyed. The whole question of the interaction of the surface state with the metal is considered in detail by V. Heine, *Phys. Rev.* (to be published).

SOFT X-RAY EMISSION SPECTRA OF AMORPHOUS PALLADIUM-SILICON ALLOY¹

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(electron bombardment; effects of crystal structure; E/T)

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This Letter presents the results of a study of L_3 valence band spectra of palladium in an amorphous palladium-silicon alloy containing 20 at. % silicon.² However, to understand the details of the valence band spectrum of the amorphous alloy, it has been found necessary to study the same spectra in pure palladium, Pd₂Si, Pd-20 at. % Si (crystalline) and Pd-H alloy. The significant new findings are: (1) a set of nondiagram satellites, hitherto unreported, shown in Fig. 1, and (2) the size, the shape, and the way the structures overlap clearly indicate their close relationship with the structure and the composition of the material, especially when the amorphous alloy transforms into the crystalline state.

A reflection-type bent-crystal vacuum spectro-

graph has been built up to ensure working facility up to about 87° Bragg angle. The L_3 valence band spectra have been studied in fifth order at an angle of about 79° using the bent mica crystal. The L_3 valence band spectrum of palladium, that is $L\beta^{2,15}$, has been studied by C. Bonnelle and C. Mande³ with bent quartz (10 $\bar{1}$ 0) in second order. They observed three satellites immediately on the short wavelength side of the main band, but did not report the presence of satellites further toward the shorter wavelength.

The ground state of the free atom of palladium is $4d^{10}$, and the solid state is represented as $4d^{9.4}5s^{0.6}$. The optical atomic levels of palladium—namely, $4d^95s$ (4 levels), $4d^95p$ (12 levels), $4d^95d$ (12 levels), etc.—begin at 0.81 eV for $4d^95s$ and terminate at