van Schilfgaarde and Newman Reply: Freeouf, Woodall, and Duke (FWD) [1] quite rightly point out aspects of our calculation that make direct comparison to experiment of limited value, many of which we addressed in our original paper. These calculations *are* well suited to address *models* of the Schottky barrier, such as the Schottky picture, which incorporate no effects beyond those contained in the calculations.

The error arising from the inverted interface for the cases Al, Ga, and Cd is much smaller than Freeouf, Woodall, and Duke suggest. There remains a high interfacial density of states at the Fermi level, even when it falls below the conduction-band edge. To show this, recalculating the Al/GaAs barrier nonrelativistically results in an interface which is no longer inverted—because the direct gap in GaAs increases by 0.65 eV—yet the barrier height increases by only 0.18 eV. This correction [2] is too small—and of the wrong sign—to affect our conclusions; see Fig. 1. Similarly, the "hydrostatic compression" of the metal was checked by recalculating Au/GaAs, stretching the Au interplanar spacings by 5%. This altered the barrier height by only 0.04 eV.

These remarks are in any case only incidental to the central question, namely, the validity of the Schottky model itself. Our position is that, owing to the large dielectric response of the interface and a high density of interface states throughout the gap, the Fermi level is constrained to lie very near the point where interface is charge neutral [3]. However, this interfacial charge-neutrality point is *not universal*, but depends on both the kind and configuration of the atoms present at the interface. Thus, we completely agree with FWD that the Fermi level for the interfaces we studied is not "pinned" in the sense that it refers to the independence of metal overlayer on barrier height. However, nor is it "unpinned" as the Schottky limit would have it. To illustrate this, we showed that the interface strongly screens out small excursions in the potential for a *given* system ($\frac{1}{120} < S < \frac{1}{30}$), "pinning" the Schottky barrier at the interfacial charge-neutrality point, in the same way that extrinsic defect levels constrain the movement of the Fermi level [3]. Our rejection of the Schottky limit does not depend on a specific choice of "internal" (or more precisely, "reference") potential [4]. For this limit to be valid, the interfacial dipole would have to be negligible. However, this dipole is prescribed by the Fermi level which makes the interface nearly charge neutral. We know of no reason why it should be small: This is the central point. Figure 1 shows that agreement with the Schottky model is poor. Whether these results are "as consistent with the Schottky model as with any other model" is really beside the point.

We had observed that relaxation of the lattice at the interface can alter the barrier height, of which the "equal pressure" condition is a special case. However, a theory that substantiates the Schottky picture must show how the lattice relaxation to a minimum-energy configuration also gives rise to a negligible dipole [5]. In a closely related problem—when two metals are joined—the dipole certainly need not be small. Now the dielectric response is infinite (as opposed to being large but finite) and thus bulk Fermi levels exactly align; the resulting dipole will be large for metals with large work-function differences.

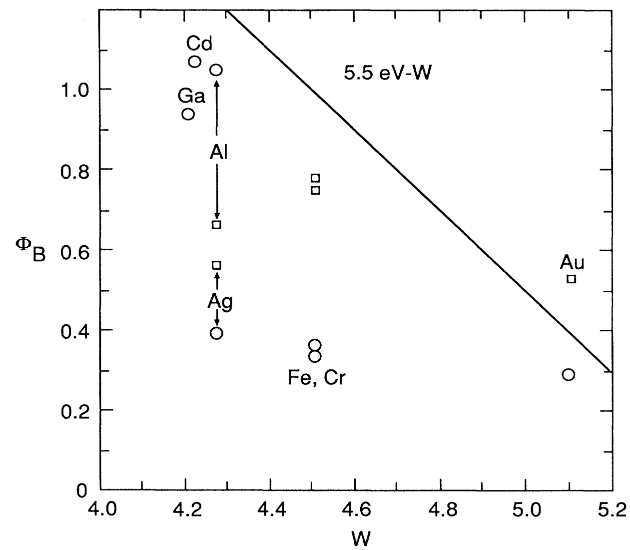

FIG. 1. Calculated (○) and measured (□) barrier heights, and the Schottky theory (——).

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[1] J. L. Freeouf, J. M. Woodall, and C. B. Duke, preceding Comment, Phys. Rev. Lett. **67**, 2745 (1991).

[2] A more serious possible source of error arises from corrections that the nonlocal exchange-correlation potential makes, even if the charge density is correct; see M. S. Hybertsen, Phys. Rev. Lett. **64**, 555 (1990).

[3] V. Heine, Phys. Rev. **138**, 1689 (1965); J. Bardeen, Phys. Rev. **71**, 717 (1947).

[4] M. van Schilfgaarde and N. Newman, J. Vac. Sci. Technol. B **9**, 2140 (1991).

[5] It is interesting to contrast the ansatz of the Schottky picture—that the dipole is negligible—to the ansatz of the neutral-point argument, that the "neutral point" is independent of the details of the metal-semiconductor interface; see F. Flores, Phys. Rev. Lett. **67**, 281 (1991).