# Summary Abstract: Schottky barrier height measurements of type A and type B $NiSi_2$ on Si

R. J. Hauenstein, T. E. Schlesinger, and T. C. McGill
*California Institute of Technology, Pasadena, California 91125*

B. D. Hunt and L. J. Schowalter
*General Electric Research and Development Center, Schenectady, New York 12301*

(Received 15 August 1985; accepted 6 December 1985)

The Schottky barrier heights of high quality MBE-grown $NiSi_2$ epi-layers on Si have been measured by photoresponse and forward $I$–$V$ methods. $NiSi_2$ is one of the few known metallic silicides which lattice matches Si and can be grown by molecular beam epitaxy (MBE) to form a nearly ideal epitaxial metal-on-semiconductor system.[1-4] $NiSi_2$ is also unique in that it can be grown epitaxially on (111) Si in two distinct orientations, designated type A and type B, with respect to the Si substrate.[1] For these reasons $NiSi_2$/Si interfaces provide a novel, well-characterized structure for the study of Schottky barrier formation, and have recently been the subject of active investigation.[1-4] At present, a controversy exists over the observed difference (greater than 0.1 eV) in Schottky barrier heights of $NiSi_2$/Si systems: On the one hand, it has been reported by Tung[2] that the barrier height depends on the *orientation* of the silicide epi-layer, while on the other hand, it has been reported by Liehr *et al.*[3] that the barrier height is independent of epitaxial orientation but instead depends on the *structural perfection* of the $NiSi_2$/Si interface. Identification of the correct dependence will have major implications for theories of Schottky barrier formation.

We have made photoresponse measurements of the Schottky barrier heights of epitaxial $NiSi_2$ on non-degenerate $n$-(111) Si substrates, for the cases of type A and type B epitaxy, on several samples with $NiSi_2$ layer thicknesses ranging from 70 to 600 Å. Nominal doping in all Si substrates was about $1.5 \times 10^{15}$ $cm^{-3}$. The photoresponse measurements were performed on broad-area-coverage regions of $NiSi_2$ on Si. No processing subsequent to growth took place on these silicide layers. Samples were illuminated from the back side (i.e., through the Si substrate) with the use of a calibrated monochromatic light source, and the open-circuit photovoltage was measured as described in Ref. 4. The crystalline quality of our type A and type B silicide layers was verified by cross-sectional transmission electron microscopy (TEM) and ion-channeling measurements, although a prominent interface peak was observed in channeling data on type B samples.[5] We consistently observe a difference in Schottky barrier height greater than 0.1 eV between type A and type B structures. At $T = 300$ K we obtain the values $\phi_{Bn} = 0.62 \pm 0.01$ eV and $0.77 \pm 0.05$ eV for the barrier heights of type A and type B $NiSi_2$, respectively, from photoresponse measurements, where an apparent barrier height correction[6] of 0.01 eV has been added to the values obtained from the conventional Fowler analysis.[7] The photoresponse curves for all type A samples exhibit linear behavior on a Fowler plot. However, photoresponse curves for all type B samples show a nearly identical deviation from the expected linear behavior at photon energies close to and below the nominal type B Schottky barrier reported by Tung.[2]

In addition to photoresponse, forward $I$–$V$ methods have also been used in the present work to determine barrier heights for type A and type B samples. Mesa structures of diameters ranging from 360 to 1300 $\mu$m were formed by a black-wax mask and etch procedure ($3HNO_3$: $1CH_3COOH$:$0.4HF$). Ohmic back contacts were obtained by painting an In–Ga amalgam on the back of the sample, though in some cases some nonlinearity in $I$–$V$ due to the back contact was observed and such samples were excluded from further consideration. A thin Au-wire probe against the silicide layer constituted the device contact. The $I$–$V$ measurements performed at $T = 300$ K yield barrier heights of $\phi_{Bn} = 0.62 \pm 0.01$ eV for type A samples in excellent agreement with the photoresponse result, with ideality factors $\eta = 1.02 \pm 0.02$. However, for type B we obtain $\phi_{Bn} = 0.69 \pm 0.01$ eV, which is considerably less than the photoresponse value (0.77 eV).

A possible explanation for both the unusual shape of the type B photoresponse curve *and* the discrepancy between electrically and optically obtained values for the barrier height is the presence of interfacial regions of mixed barrier height.[6] We have modeled our type B samples as consisting of an electrically parallel combination of regions of high and low Schottky barrier height, $\phi_{HI}$ and $\phi_{LO}$, respectively. For this model, the observed photoresponse would be an area-weighted superposition of photoresponse components from the high and low barrier regions,[6] whereas the $I$–$V$ measurement would yield a *single* mean barrier height[8] $\bar{\phi}$. We have performed a nonlinear least-squares fit of our type B photoresponse data with the use of a pair of Fowler-type functions[9] evaluated at $T = 300$ K. This fit involves three parameters—the two barrier heights ($\phi_{HI}$ and $\phi_{LO}$) and the low-barrier fractional area coverage ($\alpha$). The results of fitting to a number of type B samples of thicknesses from 70 to 600 Å consistently yields the unique set of values, $\phi_{HI} = 0.81 \pm 0.01$ eV, $\phi_{LO} = 0.64 \pm 0.01$eV, and $\alpha = 0.09 \pm 0.02$ eV. A simple calculation[8] shows that for this choice of barrier heights and coverages a forward $I$–$V$ measurement would yield a single barrier height $\bar{\phi} = 0.70$ eV, in excellent agreement with the actual observed value (0.69 eV).

In summary, our results directly demonstrate a dependence of Schottky barrier height on *orientation* of the $NiSi_2$ layer for high quality type A and type B epitaxy. We find that we confirm the results of Tung[2] but disagree with the results reported by Liehr *et al.*[3] For the case of type B epitaxy, we obtain a photoresponse barrier height from conventional Fowler analysis of $\phi_{Bn} = 0.77 \pm 0.05$ eV which is substantially greater than that of type A ($\phi_{Bn} = 0.62 \pm 0.01$ eV). A discrepancy in the measured type B barrier height between photoresponse and forward *I–V* methods, and a consistent bowing in our type B photoresponse data, are observed. However, this discrepancy, as well as the detailed shape of the type B photoresponse curve, can be quantitatively accounted for by representing the type B structure as a mixture of interfacial regions of high and low Schottky barrier height.

*Acknowledgment*: The authors wish to acknowledge the support of the Defense Advanced Research Projects Agency monitored by ONR under Contract No. N00014-84-C-0083.

[1]R. T. Tung, J. M. Gibson, and J. M. Poate, Phys. Rev. Lett. **50**, 429 (1983).
[2]R. T. Tung, Phys. Rev. Lett. **52**, 461 (1984).
[3]M. Liehr, P. E. Schmid, F. K. LeGoues, and P. S. Ho, Phys. Rev. Lett. **54**, 2139 (1985).
[4]R. J. Hauenstein, T. E. Schlesinger, T. C. McGill, B. D. Hunt, and L. J. Schowalter, Appl. Phys. Lett. **47**, 853 (1985).
[5]B. D. Hunt, L. J. Schowalter, N. Lewis, E. L. Hall, R. J. Hauenstein, T. E. Schlesinger, T. C. McGill, Masako Okamoto, and Shin Hashimoto, in Proceedings of the Materials Research Society, Boston, 1985 (to be published).
[6]T. Okumura and K. N. Tu, J. Appl. Phys. **54**, 922 (1983).
[7]S. M. Sze, *Physics of Semiconductor Devices* (Wiley, New York, 1981), p. 288ff.
[8]R. J. Hauenstein, T. E. Schlesinger, T. C. McGill, B. D. Hunt, and L. J. Schowalter, J. Vac. Sci. Technol. A (to be published).
[9]R. H. Fowler, Phys. Rev. **38**, 45 (1931).