Schottky barrier height measurements of type-A and type-B $NiSi_2$ epilayers on Si

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(Received 20 November 1985; accepted 31 January 1986)

Schottky barrier heights of single-crystal type-A and type-B $NiSi_2$ epilayers on nondegenerate n-(111) Si have been measured by photoresponse and forward $I–V$ methods. High-quality molecular beam epitaxy grown $NiSi_2$ layers of thicknesses ranging from 70 to 600 Å on sputter-cleaned, P-doped Si subtrates ($\sim 1.5 \times 10^{15}$ cm^{-3}) were studied. The type-A and type-B orientations consistently yield photoresponse barrier heights which differ by greater than 0.1 eV. We observe the value $\phi_{B_n} = 0.62 \pm 0.01$ eV for all type-A structures from both photoresponse and $I–V$ measurements. However, we obtain a discrepancy between barrier heights measured by $I–V$ ($\phi_{B_n} = 0.69 \pm 0.01$ eV) and photoresponse ($\phi_{B_n} = 0.77 \pm 0.05$ eV) methods, and in addition consistently observe an unusual bowing of the type-B photoresponse curves at low photon energies. We show that both the detailed shape of the type-B photoresponse curves and the discrepancy between $I–V$ and photoresponse-measured barrier heights can be accounted for by modeling the type-B barrier as a mixture of high and low barrier regions. Quantitative agreement with experiment is obtained for the values $\phi_{hi} = 0.81 \pm 0.01$ eV and $\phi_{lo}0.64 \pm 0.01$ eV, with effective fractional area coverages of 91% and 9% for high- and low-barrier regions, respectively.

I. INTRODUCTION

Recently, there has been much interest in single-crystal $NiSi_2$ thin films grown epitaxially on Si by molecular beam epitaxy (MBE).[1–4] $NiSi_2$ is one of the few known metallic silicides which closely lattice-matches Si ($< 0.4\%$) and can be grown by MBE to form a nearly ideal metal/semiconductor interface.[1–4] $NiSi_2$ is also unique in that single-crystal silicide layers can be fabricated on (111)-Si in two distinct orientations with respect to the Si substrate, designated type A and type B.[1] (Type-A layers are aligned exactly with the Si lattice while type-B differs by a 180° rotation about the substrate normal.) Hence, MBE-grown $NiSi_2$/Si interfaces provide us for the first time with a high-quality, well-characterized structure for advancing our understanding of Schottky barrier formation, and as such have 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 (SBH) of high quality MBE-grown $NiSi_2$/n-(111) Si systems: On the one hand, it has been reported by Tung[2] that the SBH depends on the *orientation* of the silicide epilayer, while on the other hand, it has been reported by Liehr *et al.*[3] that the SBH is independent of epitaxial orientation but instead depends on the *structural perfection* of the $NiSi_2$/Si interface. Should the SBH prove to depend on silicide orientation, the result would have major implications for theories of Schottky barrier formation,[5–7] which at present do not account for this phenomenon at a fundamental level. Even if the SBH should prove to be independent of silicide orientation, it is still of considerable practical interest to identify the origin of the reported difference in SBH results. In both studies[2,3] channeling and TEM measurements suggested high quality single-crystal $NiSi_2$ layers of either type-A or type-B orientation. However, these characterizations are not always sensitive to aspects of the *interface* region which can have a profound effect on the electrical behavior. It is therefore important to examine an independent set of SBH measurements made on samples whose fabrication details differ from those of Tung[2] and Liehr *et al.*[3] The main difference between our work and that of Tung and Liehr *et al.* was the substrate surface cleaning technique used. In our work, sputter cleaning followed by an 850 °C anneal was employed, in contrast to the higher temperature thermal cleaning methods used by Tung[2] and Liehr *et al.*[3]

In previous work[4] we have reported the observation of an orientation dependence of the SBH. We found that our SBH's as determined by photoresponse were essentially in agreement with those of Tung[2] as measured by $I–V$ and $C–V$ methods although several features of our type-B results went unresolved; in particular, the unusual shape (and hence, difficult interpretation) of the Fowler plot, and a 0.08 eV discrepancy between photoresponse and $I–V$ determined SBH In this paper we reexamine our previous photoresponse results, and supplement them with more extensive $I–V$ measurements. For type-A structures, both methods are found to consistently yield a SBH of $\phi_{B_n} = 0.62 \pm 0.01$ eV. Fo type-B samples we always observe a SBH of 0.69 ± 0.01 eV from $I–V$ measurements, and consistently see a "bowing" o the Fowler plot which was previously interpreted as corresponding to a barrier height of $\sim 0.77 \pm 0.05$ eV, where th uncertainty was mainly associated with interpretation rather than reproducibility of the result. We will show below tha both the detailed shape of the Fowler plot *and* the measured $I–V$ SBH can be *quantitatively* accounted for by modelin the type-B structure as an electrically parallel combinatio of regions of high and low barrier height.

0734-2101/86/030860-05$01.00

II. EXPERIMENTAL

A. Silicide fabrication and structural characterization

The experimental details pertinent to this work have already been discussed in detail in Ref. 4 and the reference therein, so here we limit ourselves to a brief mention of sample fabrication and characterization. In this study, type-A and type-B single-crystal $NiSi_2$ films ranging in thickness from 70–600 Å were grown by e-beam evaporation either of pure Ni or by coevaporation of Ni and Si onto type-A or type-B template layer at 650 °C. The template layers were formed following the methods developed by Tung[1,8] and annealed at 500 °C. In contrast with Tung[2] and Liehr *et al.*,[3] the Si substrates used in our work ($\sim 1.5 \times 10^{15}$ cm^{-3},P-doped) were sputter cleaned with subsequent annealing at 850 °C. Both the cleaning and film deposition steps took place in a single UHV chamber (base pressure $\sim 2 \times 10^{-11}$ Torr). The resulting $NiSi_2$ films have been extensively characterized by high-energy ion channeling, TEM, and x-ray diffraction, and show both the type-A and type-B structures to be of high quality.[9]

B. Electrical characterization

Photoresponse and forward I–V methods were used to measure the SBH of the type-A and type-B samples. The photoresponse measurements were performed by the backillumination method[10] on broad area $NiSi_2$ layers, with the use of a calibrated spectrometer. The open-circuit photovoltage was synchronously detected at levels such that $V_{ph} \ll kT$, insuring the linearity of the voltage response. The I–V measurements were made on lithographically defined devices varying between 360–1300 μm in diameter. A Au-wire probe directly on the silicide was used as the device contact in the I–V measurements presented here although it was observed that wire-bonding directly to even the thinnest (70 Å) $NiSi_2$ layers resulted in only a slight increase in leakage current. Series resistance due to the high bulk substrate resistivities necessitated numerical correction to the raw I–V characteristics, following Norde.[11] All SBH measurements were performed at room temperature.

III. RESULTS AND DISCUSSION

A. Photoresponse measurements of SBH

The results of the photoresponse measurements of SBH from our previous work[4] are summarized in Fig. 1. In this figure we present response curves taken at $T = 300$ K for typical type-A and type-B samples plotted according to the conventional Fowler analysis.[10,12] In the conventional analysis the resulting curve should contain a linear region for $(\hbar\omega - \phi_{B_n}) \geqslant 3$ kT, where $\hbar\omega$ is the photon energy, which, when extrapolated to the abscissa, gives the barrier height ϕ_{B_n} directly. As shown in Fig. 1, the type-A data can be clearly extrapolated to an intercept value of 0.61 eV. Applying an "apparent barrier height" correction (difference between ϕ_{B_n} and the extrapolated value) as discussed by Okumura and Tu,[13] we finally obtain for the type-A SBH, the value of 0.62 eV. This value is reproduced within 0.01 eV on all of our type-A samples. Turning now to the type-B photoresponse, we see from the figure that the data do not contain a clearly linear region, making conventional SBH interpretation difficult. In our previous work[4] we suggested that our type-B interfaces may contain local regions of lower SBH, resulting in the observed bowing effect in the curve at decreasing photon energies. Despite their unusual shape, our type-B photoresponse curves are quite reproducible over the full range of $NiSi_2$ layer thicknesses from 600 down to 70 Å, where one would expect the best pseudomorphic growth. Previously,[4] we have extrapolated from the upper part of the type-B curve to a SBH of 0.77 eV and quoted a rather large uncertainty (0.05 eV).

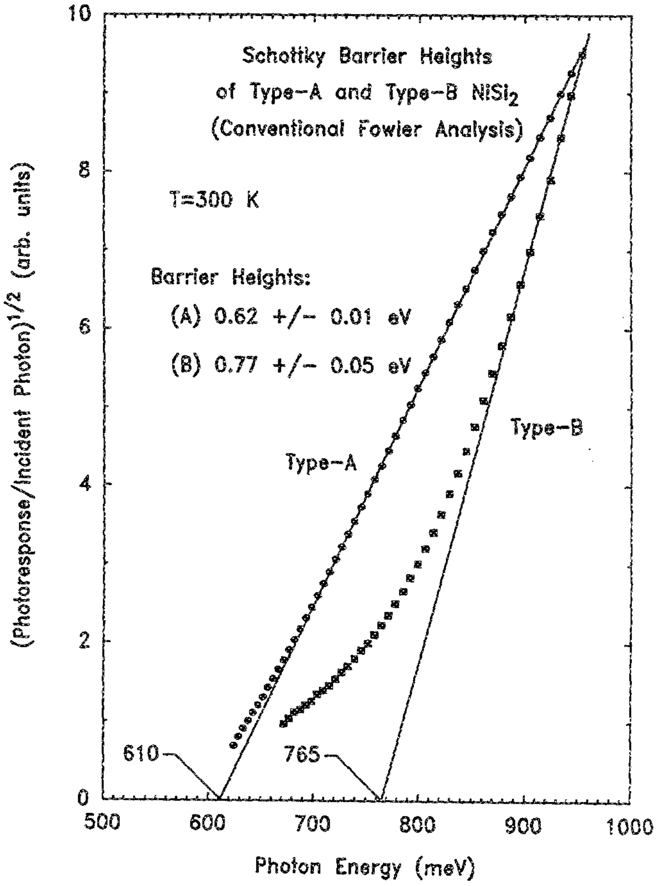

FIG. 1. Photoresponse data for $NiSi_2$/Si samples, for both type-A and type-B orientations. For clarity, data points are displayed only once every 28 actual data points. The barrier heights for type-A (250 Å) and type-B (600 Å) samples are (with apparent barrier height correction) $\phi_{B_n} = 0.62 \pm 0.01$ and 0.77 ± 0.05 eV, respectively.

B. *I–V* measurement of SBH

For comparison we have made careful forward I–V measurements of the SBH for type-A and type-B structures. These results are summarized in Fig. 2. As shown in the figure, we obtain a clear difference between type-A and type-B epitaxy. In most cases, the results (after applying a series resistance correction) are reproducible from device to device and from sample to sample within 0.01 eV, the only complication arising from samples with nonlinear back contacts, which were excluded from consideration. The excellent reproducibility of SBH and linearity over two or more

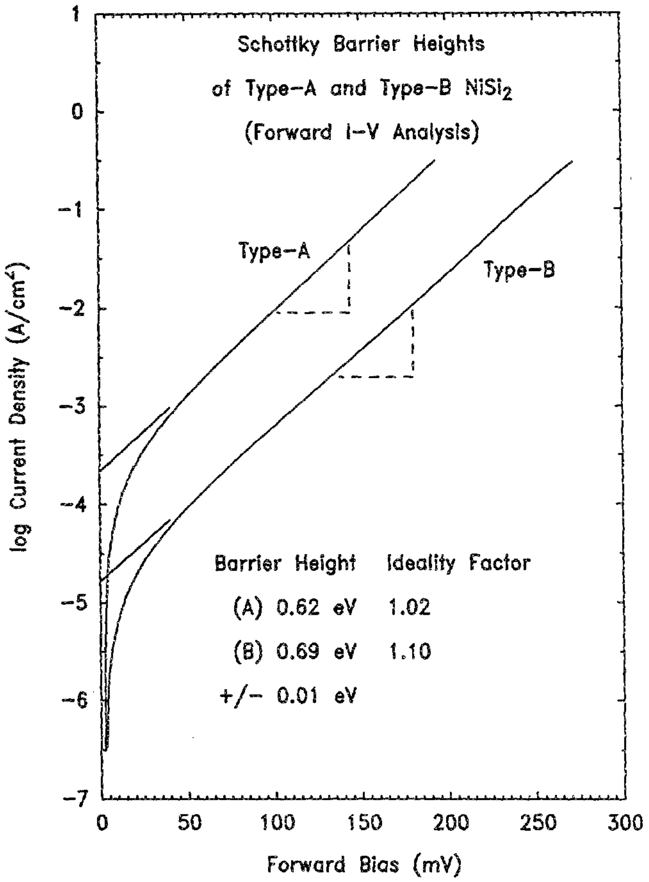

FIG. 2. Forward I–V measurements, corrected for series resistance, of Schottky barrier height for type-A and type-B NiSi$_2$/Si samples, taken at $T = 300$ K. The type-A and type-B barrier heights are 0.62 and 0.69 ± 0.01 eV with ideality factors of 1.02 ± 0.02 and 1.10 ± 0.01, respectively. A value of 110 A/cm^2 K^2 was used for the effective Richardson constant.

decades of log J vs V demonstrates the adequacy of our procedures. For type-A layers we obtain $\phi_{B_n} = 0.62$ eV with typical ideality factors $\eta = 1.02 \pm 0.02$, and for type-B we find $\phi_{B_n} = 0.69$ eV with $\eta = 1.10 \pm 0.01$.

C. Double Schottky contact model

It is clear from Figs. 1 and 2 that the type-A SBH measured by photoresponse and I–V methods are in excellent agreement, but that there is a significant discrepancy (~0.08 eV) for the case of type B. We now show that we can account for both the detailed shape of the type-B photoresponse and the observed numerical value of the I–V SBH measurement in terms of a model for the type-B interface consisting of an electrically parallel mixture of regions of high and low SBH, ϕ_{hi} and ϕ_{lo}. Okumura and Tu[13] have considered the response from compound barrier structures in detail. This analysis is based on the combined photoresponse Y of a parallel set of SBH's $\{\phi_i\}$ being given by

$$Y(\hbar\omega,T;\{\phi_j\}) = \sigma\sum_i \alpha_i C_i F(\hbar\omega,T;\phi_i), \qquad (1)$$

where $F(\hbar\omega,T;\phi_i)$ is a normalized Fowler-type photoyield function,[12] α_i corresponds to the fractional area coverage of barrier ϕ_i, σ is the active device area, and C_i is a factor which depends on the thickness, reflectivity, absorptivity, and electron attenuation length of the appropriate metal layer.[13] In our high/low barrier model we take $C_i = C =$ const and define a new normalization constant $\sigma' \equiv C\sigma$. Eq. (1) then becomes

$$Y(\hbar\omega,T;\phi_{lo},\phi_{hi}) = \sigma'[\alpha F(\hbar\omega,T;\phi_{lo}) + (1-\alpha)F(\hbar\omega,T;\phi_{hi})], \qquad (2)$$

where α refers to the effective areal fraction covered by ϕ_{lo}.

With the use of the above model we are now in a position to analyze the type-B photoresponse data. Okumura and Tu[13] have developed a general method to analyze mixed Schottky barrier structures which requires differentiation of the photoresponse curve with respect to $\hbar\omega$, which is then analyzed in terms of derivatives of Eqs. (1) or (2). However, in our work we find it both adequate and much simpler to use Eq. (2) directly. Treating the quantities, ϕ_{hi}, ϕ_{lo}, α, and σ' as adjustable parameters, we perform a least-squares fit to our experimental type-B photoresponse data using Eq. (2) evaluated at $T = 300$ K. The result is shown in Fig. 3. We see that good agreement with experiment is obtained for the values, $\phi_{hi} = 0.81$ eV, $\phi_{lo} = 0.64$ eV, $\alpha = 0.09$. We mention here that applying this fit procedure to all of our type-B samples, from 70 to 600 Å film thicknesses, yield consistency in barrier heights of ± 0.01 eV and in α of ± 0.02. In princi-

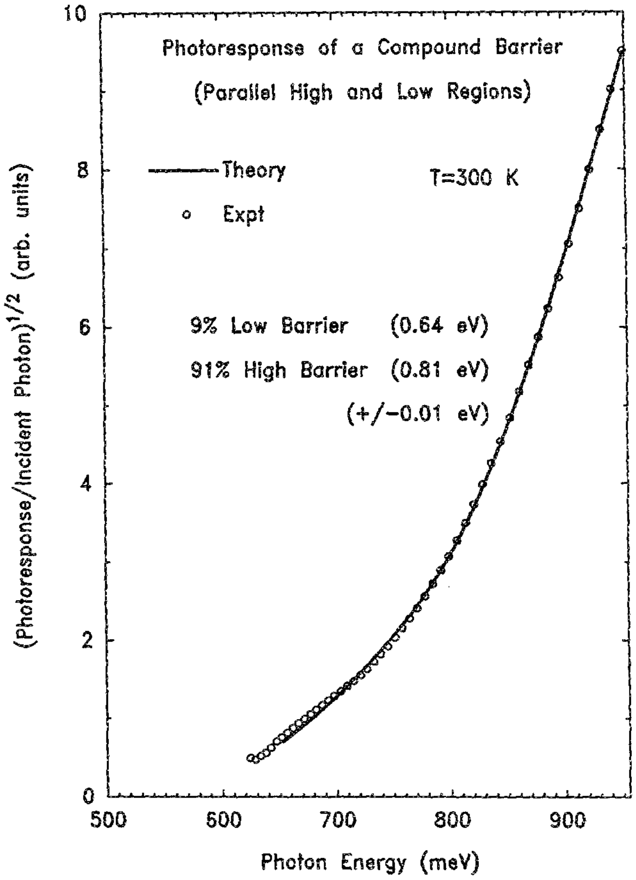

FIG. 3. Least-squares fit of the double Schottky contact model (see text) t type-B photoresponse data, at $T = 300$ K. The fit ranges over 1200 dat points, corresponding to energies covered by the solid line. The three phys cally meaningful fit parameters are the barrier heights $\phi_{hi} = 0.81$ e $\phi_{lo} = 0.64$ eV, and low-barrier areal coverage $\alpha = 9\%$.

ple, a double Schottky contact should be directly observable as a "kink" in the first derivative[13] or as a double plateau in the second derivative[14] of the photoresponse curve. However, it is straightforward to demonstrate that, for the present case, the first and second derivative spectra do not themselves yield useful information about the double contact structure at room temperature without again resorting to the type of fit described above.

Next, we use the results of the model fit to account for the observed I–V SBH for type-B samples. For parallel Schottky contacts we can define an average barrier height $\bar{\phi}$ through the expression for Schottky barrier saturation current density[10] as

$$e^{-\bar{\phi}/kT} \equiv \sum_i \alpha_i e^{-\phi_i/kT}. \tag{3}$$

Neglecting appreciable differences in ideality factors for the high- and low-barrier regions, it is the *single* SBH, $\bar{\phi}$, that would be observed in an I–V measurement. It is straightforward to show that, for the present case, Eq. (3) leads to the expression

$$\bar{\phi} \approx \phi_{\mathrm{lo}} - kT \ln \alpha, \tag{4}$$

valid whenever $\alpha \exp[(\phi_{\mathrm{hi}} - \phi_{\mathrm{lo}})/kT)] \gg 1$. Using the values of $\phi_{\mathrm{hi}}, \phi_{\mathrm{lo}}$, and α obtained from the model fit above yields $\bar{\phi} = 0.70$ eV, in excellent agreement with the type-B SBH directly measured by the I–V method (0.69 eV). It is easy to show that taking proper account of the ideality factors leads to a correction term in Eq. (4) of $\approx -qV(\Delta\eta/\bar{\eta}^2)$, where qV is the forward bias (in eV), $\bar{\eta}$ is the mean ideality factor, and $\Delta\eta$ the difference between the low-barrier ideality factor and $\bar{\eta}$. From this we see that neglecting the ideality factors leads to an error of less than 0.01 eV for reasonable values of the ideality factors. Thus, with a simple model we have shown quantitative consistency between apparently disparate SBH results for the case of type-B $NiSi_2$ layers measured by two different methods.

D. Interpretation

The interpretation of our photoresponse and I–V SBH measurements suggest that most (91%) of the interfacial area of our type-B $NiSi_2$/Si structures is associated with a SBH of 0.81 eV, but also present are localized regions, comprising 9% of the effective device area, that are associated with a reduced barrier height, 0.64 eV. There are two possibilities that immediately spring to mind to account for this phenomenon. Noting that the value of ϕ_{lo} is close to the type-A SBH, it may be that simultaneously present at the $NiSi_2$/Si interface are grains of type-A orientation mixed in among the type-B structure. This possibility is discounted by our channeling and TEM observations, however, which show both our type-A and type-B films to be of comparable quality. A second possibility is that localized interfacial structural disorder gives rise to localized electronic states of sufficient density to locally pin the Fermi level. Dislocations are observed[9] in plane view TEM images of type-B $NiSi_2$ while none are observed in type-A films over the range of thickness reported here. However, since the density of dislocations increases with increasing type-B film thickness, the consistent observation of bowing in the photoresponse for all type-B layers argues against misfit dislocations as the cause. It is possible that the low barrier height regions may be associated with the localized *planar* defects seen in high resolution TEM, as discussed in Ref. 9. At the present time the case of these planar defects is not understood and is under investigation. Finally, the absence of any nonideality in the physical or electrical characterization of the type-A structures and the significant difference between type-A and type-B measured barrier heights would suggest the absence of some foreign surface contaminant which dominates the electrical behavior near the interface.

IV. SUMMARY

In summary, we have made Schottky barrier height measurements on high-quality, MBE-grown $NiSi_2$/Si structures of type-A and type-B orientations with the use of photoresponse and forward I–V techniques. Comparison of the data obtained from both techniques clearly demonstrate a difference in barrier heights between type-A and type-B structures. This finding is in agreement with the results of Tung[2] but in disagreement with the results of Liehr *et al.*[3] The main contribution from this paper is the side-by-side comparison of photoresponse and I–V measurements made on the *same* samples, and the unique comparison that these complementary measurements allow. For the case of type-A epitaxy, we consistently obtain a barrier height from both techniques of $\phi_{\mathrm{B}_n} = 0.62 \pm 0.01$ eV. For the case of type-B, a serious discrepancy in the barrier height between photoresponse and forward I–V methods is observed. Furthermore, the qualitative shape of the type-B Fowler plots are nonlinear but consistent from sample to sample, rendering determination of barrier height ambiguous. We have shown that both the detailed shape of the Fowler plot as well as the measured I–V value of type-B barrier height for our samples can be quantitatively accounted for in terms of a double Schottky contact model. In this model, the type-B structure consists of electrically parallel regions of high and low barrier height, where $\phi_{\mathrm{hi}} = 0.81 \pm 0.01$ eV, $\phi_{\mathrm{lo}} = 0.64 \pm 0.01$ eV, with the effective area of low- and high-barrier coverages being 9% and 91%, respectively. The possible physical realizations of this model within the $NiSi_2$/Si system are discussed.

ACKNOWLEDGMENTS

The authors wish to acknowledge the support of the Defense Advanced Research Projects Agency monitored by ONR under Contract No. N00014-84-C-0083. One of us (R.J.H.) received financial support from IBM and another one of us (T.E.S.) from GTE. We also wish to thank Masako Okamoto and Professor W. M. Gibson from SUNY Albany for ion channeling RBS measurements. Dr. E. L. Hall and N. Lewis of the GE Crop. R&D Center are also gratefully acknowleged for their TEM work on these samples. Finally, the expert technical assistance of L. Turner in operating the MBE system is acknowleged.

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