Schottky-Barrier Inhomogeneity at Epitaxial NiSi$_2$ Interfaces on Si(100)

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The Schottky-barrier height (SBH) of an epitaxial NiSi$_2$ layer grown on Si(100) is shown to depend critically on the morphology of the interface. Single-crystal, uniform, planar NiSi$_2$/Si(100) layers have a much lower (*n*-type) SBH than that of interfaces which are made up of inclined $\langle 111 \rangle$ facets. Interfaces with both planar $\langle 100 \rangle$ sections and inclined $\langle 111 \rangle$ sections exhibit electrical behavior expected of a spatially inhomogeneous SB. We suggest that interface atomic structure determines SBH formation.

The formation mechanism of Schottky barriers at metal-semiconductor (MS) interfaces has puzzled scientists for decades.[1,2] Presently, the most popular theories involve Fermi-level (FL) pinning by either defect states[3,4] or by states derived from the semiconductor.[5] Significantly, the FL pinning mechanism does not have a first-order dependence on atomic structure of the MS interface. However, recent measurements of the electronic properties of high-quality, epitaxial MS interfaces tend to show otherwise.[6-9] For example, the NiSi$_2$ Schottky-barrier height (SBH) on *n*-type Si(111) is 0.65 eV for type-*A* orientation and 0.79 eV for type-*B* orientation.[6,7,10] This difference in SBH has been reproduced in recent calculations which support the notion that interface atomic structure plays a crucial role in determining SBH.[11,12] In this paper, new results from epitaxial NiSi$_2$/Si(100) structures are presented which link measured inhomogeneous interface structure to measured electrical properties. In contrast to the popular view, our work suggests an intrinsic SB formation mechanism based on local interface atomic structure.

If one considers the possibility that SBH depends on interface structure, then at MS interfaces whose atomic structure varies from region to region, so should the local FL position. Indeed, evidence from ballistic electron emission microscopy[13] (BEEM) studies suggest the existence of local SBH variations. The difference between SBH measured by a current-voltage (*I-V*) method and that measured by a capacitance-voltage (*C-V*) method is also evidence for SBH inhomogeneity.[6,14] However, at present, there is no adequate theory of a spatially inhomogeneous SBs electrical characteristics. Existing treatments[15] fail when the FL varies on a scale less than, or comparable to, the width of the semiconductor depletion region.[16,17] Since the FL at a NiSi$_2$/Si(100) interface often varies laterally on a length scale < 100 Å, care must be taken to ensure a correct solution to Maxwell's equations is obtained before interpreting *I-V* and *C-V* data.[18]

A variety of *n*- and *p*-type $\langle 100 \rangle$-oriented Si substrates, ranging in impurity concentration from 1×10^{15} to 1×10^{17} cm^{-3}, are used in these studies. Routine *ex situ* and *in situ* cleaning procedures[19] are used to obtain clean reconstructed surfaces in a Si molecular-beam-

epitaxy chamber. NiSi$_2$ layers, 40–200 Å thick, with a wide variety of interface morphologies are grown according to previously described techniques.[20] A 100–200-Å-thick Co "cap" layer is deposited on the portion of the NiSi$_2$ samples used for SBH investigation. Grown silicide samples are cleaved in half for structural and electrical characterization, respectively. Plan-view transmission electron microscopy (TEM) and Rutherford-backscattering analysis are performed on most of the NiSi$_2$ layers.

To facilitate electrical measurement, Ohmic contact is made to the back side of the samples. Arrays of approximately square mesa diodes, ~1000 Å in height, are processed by photolithography and wet and dry etching. Further metallization by Co/Ti/Au is achieved using a liftoff procedure. Diodes have areas ranging from 1 $\times 10^{-4}$ to 1×10^{-2} cm^2. *I-V* and *C-V* measurements are made in a shielded dry box with the ambient temperature adjustable from −100 to 100 °C. The diode current is always studied as a function of diode size to avoid possible influence of edge leakage current. Forward saturation currents are obtained to deduce Φ_B,[1,21] using 112 and 32 A K^{-2}cm^{-2} as Richardson's constant for *n*- and *p*-type Si, respectively. Barrier lowering due to image force is calculated and used to determine the flat-band SBH, Φ_B^0. To minimize parallel conductance, capacitances are usually measured at below room temperature.[22] Φ_B^0 is determined by extrapolation of C^{-2}.[1,21]

NiSi$_2$ has the CaF$_2$ crystal structure and a good lattice match to Si. Interfaces between NiSi$_2$ and Si(100) frequently contain sections of inclined $\langle 111 \rangle$ facets in the form of narrow "bars" of NiSi$_2$ inclusion.[23] Typically, "facet bars" have widths of ~50–100 Å and are over 500 Å in length. They are clearly seen under (002) dark-field TEM imaging as the bright streaks shown in Fig. 1(b). SBH of epitaxial NiSi$_2$ layers on Si(100) was briefly reported a few years ago.[24] However, the poor quality of the material and the ever present facet bars prevented the determination of the SBH associated with planar NiSi$_2$/Si(100) interfaces. Recently, it was discovered that codeposition of NiSi$_2$ and a high-temperature (> 700 °C) anneal completely eliminate the presence of facet bars and significantly reduce the density of disloca-

FIG. 1. Plan-view, (002) dark-field, TEM images of ~80-Å-thick $NiSi_2$ layers grown on Si(100). A facet bar shows up as a bright streak under this imaging condition. Dark lines are defects with $\frac{1}{4}$ (111) character, which decorate steps with an odd number of atomic planes at the interface. (a) A layer which is nearly completely faceted. (b) A layer with mixed morphology. (c) A uniform layer.

tions,[20] as illustrated in Fig. 1(c). Also, growth techniques to fabricate $NiSi_2$/Si interfaces which are nearly completely faceted, such as the one shown in Fig. 1(a), are known.[20] An examination of the $NiSi_2$ layers displayed in Fig. 1 clearly indicates the wide range of interface morphologies accessible by existing growth methods.

There is a strong correlation of SBH characteristics with the observed interface morphologies. At least three samples from each doping and morphology category were grown and an average of eight diodes were studied from each sample. Interfaces which are almost completely ⟨111⟩ faceted have SBHs similar to that found at a type-A $NiSi_2$/Si(111) interface, as shown in Table I. SBHs of $NiSi_2$ layers were found to be independent of the film thickness. I-V plots from such interfaces have excellent ideality factors, $n \leq 1.03$, on both n- and p-type Si. C-V measurements yielded SBHs which are slightly larger, ~0.05 eV, than those measured by the I-V method. We note that the SBH observed from heavily faceted interfaces is in good agreement with that reported by Kikuchi, Ohshima, and Shiraki,[25] who used a growth technique which is known to lead to almost completely faceted interfaces.[20] Inclined facets at the $NiSi_2$/Si(100) interface are simply sections of a type-A $NiSi_2$/Si(111) interface. It is not surprising that the SBH found for a $NiSi_2$/Si(100) interface entirely made up of facets is identical to that found at a planar type-A

$NiSi_2$/Si(111) interface.[6]

The electrical characteristics of uniform $NiSi_2$ layers on Si(100) are summarized in Table II. On n-type substrates, ideality factors for I-V measurements are good ($n < 1.03$) and very consistent results were obtained. Typical C-V results are shown in Fig. 2. On p-type Si(100), current through the smaller diodes is low and the total current becomes dominated by edge leakage current at temperatures below ~0°C. Therefore, I-V measurements for p-type SB were made at, or above, room temperature. I-V traces are characterized by ideality factors $n \geq 1.08$. SBH results showed some slight variations on p-type Si. On lightly doped p-type Si, I-V and C-V studies yielded SBHs which are in good agreement. With an increase of the doping level, there is a slight decrease of the I-V determined SBH and a slight increase in the C-V determined SBH. A possible origin of this dependence will be discussed later.

The low SBH of ~0.4 eV measured from uniform $NiSi_2$ layers is very different from the value 0.6–0.7 eV usually observed for polycrystalline nickel silicides on n-type Si(100).[26] Presently, the proposed atomic structure of the flat $NiSi_2$/Si(100) interface is the sixfold-coordinated model.[27,28] Since the $NiSi_2$/Si(100) interface has an entirely different atomic structure from either of the two $NiSi_2$/Si(111) interfaces, it is perhaps not surprising that the SBH is also different. For example, the SBH of 0.79 eV for type-B $NiSi_2$ on n-type Si(111) exceeds the present $NiSi_2$/Si(100) SBH by ~0.4 eV (more than one-third of the Si band gap). This giant variation of FL position between the same metal and semiconductor cannot be explained by FL pinning due to either defect states or the mechanism proposed by Tersoff.[5] An intrinsic mechanism based on the interface atomic structure is strongly suggested.

The presence of a few facet bars at $NiSi_2$/Si(100) interfaces which are otherwise flat has little effect on n-type SBH, but has a strong influence on the measured SBH of p-type Si. The I-V deduced p-type SBH decreases rapidly as the density of facet bars increases, while a slower, but noticeable, decrease of the C-V SBH is concurrently observed. As a result, the C-V measured SBH for any specific diode significantly exceeds that deduced from I-V. Mixed-morphology p-type diodes are

TABLE I. Schottky-barrier heights of heavily faceted $NiSi_2$ on Si(100).

Silicon	Doping (cm^{-3})	$\Phi_B^0 (\pm 0.02$ eV)	
		I-V	C-V
n-type	1.5×10^{16}	0.65	0.68
	1.6×10^{15}	0.65	0.67
p-type	1×10^{17}	0.43	0.50
	3.6×10^{16}	0.44	0.49

TABLE II. Schottky-barrier heights of uniform $NiSi_2$ on Si(100).

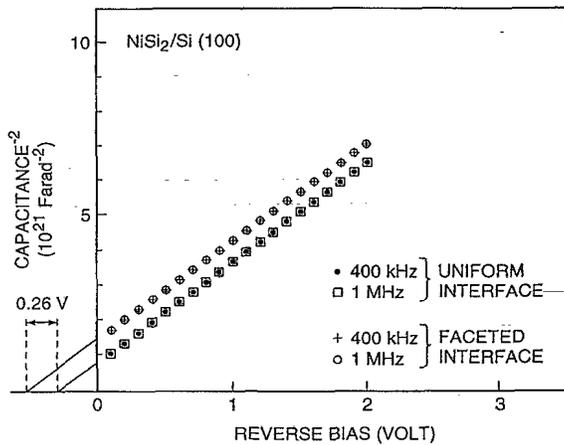| Silicon	Doping (cm^{-3})	$\Phi_B^0 (\pm 0.02$ eV)	
		I-V	C-V
n-type	5×10^{16}	0.38	0.40
	1.5×10^{16}	0.41	0.42
	5×10^{15}	0.40	0.37
	1.6×10^{15}	0.40	0.39
p-type	1×10^{17}	0.68	0.77
	3.6×10^{16}	0.72	0.77
	5×10^{15}	0.73	0.74

FIG. 2. Capacitance-voltage plots of NiSi$_2$ layers on 1.6×10^{15}-cm^{-3} phosphorous-doped (n-type) Si(100). Measurements are performed at $T = 198$ K at frequencies of 400 kHz and 1 MHz. Diode area is 1.6×10^{-3} cm^2.

"leaky," having poor ideality factors $n \geq 1.1$ in forward bias and displaying reverse currents which do not saturate. There is also a clear dependence of the electron transport on the substrate doping level. As an example, NiSi$_2$ layers with similar densities of facet bars, but grown on p-type Si with different doping levels, have been selected and their electrical properties shown in Table III. The C-V determined SBHs of these layers are similar, but the SBH deduced from I-V analysis decreases rapidly with increasing doping level.

Since the SBH associated with a flat NiSi$_2$/Si(100) interface is different from that of inclined $\langle 111 \rangle$ facets, an interface consisting of both structures is electrically inhomogeneous. Existing treatments of SBH inhomogeneity assume the various "patches" of different local SBHs to be noninteracting.[15] Thus, the total current is a simple sum of individual currents flowing in different patches of the junction. This approach is incorrect because when patches are smaller than, or comparable to, the space-charge region width, electron transport in each individual patch can no longer be treated as independent, even in the classical regime. Conceptually, this is easy to understand: Small areas with low SBH are easily "pinched off," if surrounded by regions with high SBH. The current arriving at a low-SBH patch thus depends on the height of the "saddle point" in front of it, and not

TABLE III. SBH of NiSi$_2$ layers on p-type Si(100) which have similar interface morphologies. Facets occupy $\sim 10\%$ of the total area.

Doping (cm^{-3})	Expt. (eV) Φ_B^0 (C-V)	Expt. (eV) Φ_B^0 (I-V)	Calc. I-V Φ_B^0 (eV) Saddle point	Calc. I-V Φ_B^0 (eV) Ref. 15
1×10^{17}	0.73	0.50	0.52	0.52
3.6×10^{16}	0.74	0.60	0.59	0.52
5×10^{15}	0.73	0.64	0.68	0.52

the local SBH at the MS interface.[16,18] Only when patches are very large, or the doping level is very high, may the electrical transport from different patches be treated as independent. When pinchoff occurs, it is clear that the two relevant parameters governing the transport of charge to and from the individual patches are the "effective SBHs" Φ_{eff}, which are just the saddle-point minima, and the "effective areas" of the patches, A_{eff}. Simply put, the total forward current is a sum of individual currents flowing in different effective areas,

$$ I(V) = A^{**} T^2 e^{qV/kT} \sum_i e^{-q\Phi_{\text{eff}}^i/kT} A_{\text{eff}}^i , \tag{1} $$

where the symbols have their usual meanings. Recently, analytic expressions for the saddle-point minimum and the effective area have been derived.[18] Since the potential field depends on the applied bias, an ideality factor larger than unity is a consequence of an inhomogeneous barrier height where the current is dominated by transport through isolated "hot spots."[18] This originates from the increase in height of the saddle points as the forward bias increases. It is also clear that the lower the doping level, the higher the measured "apparent SBH" from I-V, and the more uniform the electrical junction appears to be. Conversely, the most information on SBH inhomogeneity is obtained from more heavily doped substrates. Pinchoff also affects current transport in reverse bias. A decrease of Φ_{eff} leads to an increase in current with increasing reverse bias. In passing, we note that, because of pinchoff, the apparent profile obtained by BEEM (Ref. 13) is not a contour of the interface FL position, as previously thought.

Based on the above, the SBH data from NiSi$_2$ layers of mixed-interface morphology may be qualitatively understood. We may assign a local n-type Φ_B^0 of 0.65 eV (0.44 eV on p-type Si) to areas occupied by facet bars and 0.40 eV (0.72 eV on p-type Si) to the flat areas. Since flat areas usually occupy the majority of the interface in a mixed-morphology film, an almost constant SBH is observed by I-V on n-type Si. On a p-type substrate, almost all the current originates from the small, isolated facet bars which are partially pinched off. A consequence of this inhomogeneity is the observed strong dependence of the measured I-V SBH on the density of the facet bars and doping level. The high ideality factors and increasing reverse currents are also consistent with this scenario. Although the qualitative behavior of an inhomogeneous SB is predictable,[18] quantitative analysis of electrical data is difficult, even with the aid of TEM. This is because the saddle-point potential depends not only on the size, but also on the shape of each individual patch. At a real NiSi$_2$ interface, there is a large distribution of the length and width of the facet bars. Furthermore, the physical protrusion of a facet bar into Si lowers the saddle-point potential. However, as a rough estimate of the I-V behavior, we shall assume a single saddle-point minimum for all the low SBH patches.

Based on the observed average width of larger facet bars, ~ 150 Å, and typical areal density of 10%, the saddle-point potential may be evaluated as a function of the doping level and the expected I-V behavior calculated. The saddle-point calculation qualitatively reproduced the dependence on doping level, as shown in Table III. If no interaction between patches is assumed, as in Ohdomari and Tu's[15] analysis, the experimentally observed dependence on doping level is inexplicable.

As for flat $NiSi_2/Si(100)$ interfaces, examination of the I-V results reveal a dependence on p-type doping level (see Table II). From earlier discussion, this is an indication of SBH inhomogeneity. The contribution from tunneling is negligible at these doping levels. Therefore, $NiSi_2/Si(100)$ interfaces, even those which appear perfectly uniform to plan-view electron microscopy, are likely microscopically inhomogeneous. The origin of this SBH inhomogeneity is possibly related to the partial 1×2 reconstruction which has been shown to be present at this interface.[20] Streaked intensity at the $\langle \frac{1}{2} \frac{1}{2} 0 \rangle$ positions were routinely observed, by electron diffraction, in thin $NiSi_2$ layers. These diffracted beams originate from long "chains" of reconstructed regions. The structure of the partial reconstruction at the $NiSi_2/Si(100)$ interface is unknown, although it is probably similar to the strong 1×2 reconstruction seen at the $CoSi_2/Si(100)$ interface.[29,30] In any event, the local interface structure at a reconstructed region must be quite different from that in an unreconstructed region. We speculate that this difference in the interface atomic structure is the origin of the observed SBH inhomogeneity at flat $NiSi_2/Si(100)$ interfaces.

In the published literature on (mostly polycrystalline) MS junctions, there are numerous examples of the observation of a SBH dependence on the doping level or on the method of measurement. Another frequent encounter in SBH studies is the observation of a poor ideality factor in I-V measurement. The existence of interface states has been the most popular explanation of such anomalies. We find it quite surprising that barrier height inhomogeneity has thus far not even been mentioned as a likely explanation of all these phenomena. A possible reason for this glaring omission is an apparently deep-rooted belief that FL pinning must be uniform across the entire MS interface. Recent experimental results, including those presented here, suggest such a view should be critically reassessed. Our results suggest the physics controlling Schottky-barrier formation depends on the spatially *local* metal-semiconductor interface atomic structure.

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