SAND99-0594J

Silicide Schottky Contacts to Silicon: Screened Pinning at Defect Levels

Timothy J. Drummond
Sandia National Laboratories
Albuquerque, New Mexico 87185-0603

ABSTRACT

Silicide Schottky contacts can be as large as 0.955 eV (E_v + 0.165 eV) on n-type silicon and as large as 1.05 eV (E_c - 0.07 eV) on p-type silicon. Current models of Schottky barrier formation do not provide a satisfactory explanation of occurrence of this wide variation. A model for understanding Schottky contacts via screened pinning at defect levels is presented. In the present paper it is shown that most transition metal silicides are pinned approximately 0.48 eV above the valence band by interstitial Si clusters. Rare earth disilicides pin close to the divacancy acceptor level 0.41 eV below the conduction band edge while high work function silicides of Ir and Pt pin close to the divacancy donor level 0.21 eV above the valence band edge. Selection of a particular defect pinning level depends strongly on the relative positions of the silicide work function and the defect energy level on an absolute energy scale.

INTRODUCTION

There have been a large number of papers published which have attempted to systematize Schottky barrier contacts to silicon. Correlations between the barrier height and the silicide heat of formation[1, 2], work function[3], core level shifts[4], and Miedema electronegativity[5, 6] have been explored. Other works have proposed defect pinning models[7-9]. In the present work it is demonstrated that defect pinning is the dominant mechanism. Selection of the defect which determines the barrier height is sensitive to the work function of the silicide contact. Furthermore, the measured barrier height does not pin exactly to the defect level as charge transfer from, or to, the silicide is screened at the interface. A model for screened pinning at defects has recently been developed and applied successfully to Schottky contacts to GaAs[10]. The same model is applied to silicon to identify divacancy levels, vacancy clusters and interstitial clusters as pinning levels for silicide Schottky contacts to silicon.

The central feature of the present investigation is a model for Schottky barrier contacts which emphasizes the role of near surface defects in determining the Schottky barrier height. "Near surface" implies that the defects are within a decay length of the silicide electron wave function into the silicon at the interface. Defects within this region form resonant bonds with the silicide. If the defect density is sufficiently large the interfacial charge dipole set up between the silicide and the defect resonance in the silicon determines the Schottky barrier height. Application of the model requires a data set describing silicide barrier heights to silicon, knowledge of the silicide work functions, and the energy levels of defects and defect clusters in silicon.

A new silicide barrier height data set was compiled for the present

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, make any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

work. Most previous attempts to understand silicide/silicon Schottky barrier heights refer to review papers (see for example [11]) for the "characteristic" barrier heights of silicide contacts. Ultimately these review papers trace the majority of these values to an early paper by Andrews and Phillips [1] who cite Schottky barrier values for a number of silicide contacts to n-Si referring to unpublished work for details of fabrication. This has been largely accepted due to the assertion that specific silicide contacts yield highly reproducible barrier heights. Examination of the subsequent literature shows process dependent variation over a range as large as 0.18 eV and dependent on process history. This is especially true of low work function silicides. While high work function silicides are less process dependent the belief that all silicides have a unique barrier height must be revised.

The second essential component of the analysis is the availability of good work functions for the silicides. The values used in the present work are computed from the metal and silicon work functions using an average charge transfer model[12]. The work functions of the metallic elements from rows three through six of the periodic table were reviewed. Experimental silicide work function data were compiled and compared with theoretical prediction. For those metals whose work function was greater than that of silicon excellent agreement between theory and experiment was found. For the metals with work functions less than the silicon work function the silicides separated into two groups, one containing rare earths and one containing transition metals. In each group it appeared that a surface effect systematically increased the linear slope relating the experimental work function relative to the theoretical value. In the present work it is assumed that the average charge transfer theory correctly predicts the "bulk" silicide

work function as appropriate to the application of the screened pinning model for the barrier height.

Finally, the credibility of the model depends upon being able to successfully correlate Schottky barrier data with known defect energy levels. The model is able to distinguish between donor (hole trap) and acceptor (electron trap) type defects. While several studies of radiation and implantation induced defects were considered[13-27] it was found that the data could be explained in terms of the accepted divacancy (V_2) levels, ensemble vacancy (V_n) and silicon interstitial (I_n) cluster levels[28-33]. Unless specifically noted the silicide contacts considered were formed by the deposition of an elemental metal on a silicon surface followed by an anneal sequence. The end product is typically a polycrystalline silicide in contact with the silicon. Since a substantial amount of silicon is consumed in the silicidation the silicide interface is assumed to be clean although impurities may be snowplowed ahead of the reaction front or oxygen may diffuse to and accumulate at the interface. Neglecting impurity effects, it is assumed that silicidation does generate a high concentration of intrinsic defects within a few nanometers of the interface which ultimately determine the Schottky barrier height.

THEORY

The model for screened pinning at defects has been described previous in the context of Schottky contacts to GaAs[10]. In the absence of defects a Schottky barrier height would be determined by the Fermi level in the metal and the intrinsic chemical potential of the semiconductor. Bond charge transfer at the interface tries to align the two level. Perfect alignment is not

achieved as charge transfer is limited by screening. The strength of the screening is a function of the interfacial permittivity which is in turn determined by the individual bulk permittivities of the two materials brought into contact as

$$1/\varepsilon_i = [1/\varepsilon_\infty(A) + 1/\varepsilon_\infty(B)]/2 \qquad (1)$$

Assuming that the silicide is metallic and approximating its permittivity as infinite the interfacial permittivity is simply $\varepsilon_i = 2\varepsilon_\infty(Si)$. With this definition of the interfacial permittivity the intrinsic silicide barrier on n-type Si would be

$$\phi_{bn} = \phi_{bn,SM} + [\phi^* - \phi_{mSi}]/(1 - 1/\varepsilon_i) \qquad (2)$$

where ϕ^* is the intrinsic chemical potential of Si relative to the vacuum level, ϕ_{mSi} is the metal silicide work function and $\phi_{bn,SM}$ is the Schottky-Mott barrier height. The Schottky-Mott barrier is the difference, ϕ_{mSi} - A, between the silicide work function and the electron affinity of silicon. Assuming a room temperature band gap of 1.12 eV for Si the electron affinity is A = 3.90 eV. Defining an intrinsic barrier height as $\phi_{bn}^* = \phi^* - A$, Equation 2 may be rewritten as

$$\phi_{bn} = \phi_{bn}^* + [\phi_{bn,SM} - \phi_{bn}^*]/\varepsilon_i. \qquad (3)$$

In this format Equation 3 is similar to the expression presented in the ViGS/MIGS model for Schottky barrier heights[34]. In fact, ϕ_{bn}^* locates the charge neutrality level, as defined by those models, relative to the conduction band edge. The difference is in the form of the screening factor which appears here simply as $\varepsilon_i = 2\varepsilon_\infty(Si)$. In the case of a nonideal interface the measured barrier height is determined by aligning a defect level within the Si band gap to the silicide Fermi level. If the defect level is located relative to the vacuum level as E_{pin} (as it pins the interface Fermi level) define the unscreened defect

pinned barrier as $\phi_{bn}' = E_{pin} - A$. The final result for screened pinning at a defect level is obtained by substituting ϕ_{bn}' for ϕ_{bn}^* in Equation 3.

For Equation 3 to be applied it must be true that ϕ_{mSi} locates the silicide Fermi level relative to the vacuum level and that ϕ^* locates intrinsic chemical potential of silicon relative to the vacuum level. In prior work it has been argued that the surfaces of "good" polycrystalline metals characteristically have a zero net surface dipole and that the polycrystalline work function of a metal does indeed locate the Fermi level relative to the vacuum[12, 35]. In the same context the polycrystalline work function of Si was estimated to be $\phi^* = 4.66$ eV. The error in this valuation is believed to be on the order of $\pm$ 0.05 eV. Experimental values for the work functions of metal silicides were compiled and compared with the predictions of an average charge transfer (ACT) model[12]. The ACT model is similar in spirit to the screened pinning model for Schottky barrier formation in that electronegativity equalization is screened by a factor derived from the atomic polarizability (the analog of the permittivity). Excellent agreement was obtained for silicides formed from metals with work functions ϕ_m greater than ϕ^*. This group includes most of the late transition metals. For metals with $\phi_m < \phi^*$ a linear correlation was found to hold separately for the rare earth elements and the early transition metals. For both groups the slope was identical and greater than the slope predicted by the ACT model. This behavior was proposed to be a surface phenomena of compounds comprised of one metallic element and one covalent element. In this work it will be assumed that the theoretical ACT work function of the transition metal silicides properly locates the bulk chemical potential. While this assumption cannot be rigorously justified it will be shown to be entirely consistent with the interpretation of the data. Furthermore, a large number of

technologically relevant silicides fall in the group $\phi_m > \phi^*$ and are not affected by this assumption.

In the formation of silicide contacts metals are deposited on silicon and annealed at temperatures which are typically greater than 300 °C. This temperature is sufficient for both vacancies and interstitial silicon to agglomerate into clusters. Assuming that the silicidation process generates a large number of intrinsic defect near the reaction front it is reasonable to expect cluster defects to play an important role in controlling the barrier height. While there are several papers describing the properties of point defects produced by radiation damage in silicon the references found to be most valuable to the present work describe cluster defect levels detected in Si self-ion implantation and annealing studies[28-33]. The primary defect involved in Schottky barrier pinning appear to be an interstitial cluster ensemble, I_n, at E_v + 0.48 eV. This level behaves as a donor (hole trap). The second most important defect is the divacancy V_2. For low work function silicides, particularly the rare earth silicides, the Schottky barrier is pinned close to the V_2 acceptor level at E_c - 0.41 eV. For the very high work function silicides of Ir and Pt the Schottky barrier pins close to the V_2 donor level at E_v + 0.21 eV. Vacancy clusters, V_n, have been correlated with ensemble acceptor level located at E_c - 0.55 eV. Evidence for pinning at either V_2 or V_n, depending upon processing history is evident in the data to be presented.

The clusters pinning the Schottky barrier height are visualized as being roughly planar with n less than 10[15, 36, 37]. Identifying them with bulk cluster levels is problematic as the formation kinetics and stability of these levels is certainly affected by their close proximity to the silicide/silicon interface. Near surface vacancies are introduced at Si(111)-7×7 surface annealed above 700 °C to relive strain[38]. Subsurface interstitials are known

to stabilize the Si(113)-3×2 surface[39]. These defects have also, by assumption, formed resonant bonds with the silicide although the defects have no metal atoms as first nearest neighbors. This feature appears to allow the defect to retain much of its bulk character in silicon as well as in GaAs. The fact that they are coupled to the silicide does appear to render them less susceptible to hydrogen passivation that free clusters/defects further from the interface which do not couple to the evanescent silicide wave functions.

DISCUSSION

Application of the screened defect pinning model is illustrated in Figure 1. The experimental data points are shown as triangle and squares for contacts to (111) and (100) silicon surfaces, respectively. Schottky barrier heights to n-type Si, ϕ_{bn}, are shown as solid symbols while Schottky barriers to p-type silicon are shown as open symbols representing the equivalent n-type barrier computed as $(E_g - \phi_{bp})$. The horizontal scale is the silicide work function which nominally locates the silicide work function relative to the vacuum level. The vertical dashed lines locate the Si conduction and valence band edges relative to the vacuum level. The valence band edge is placed at 5.02 eV as determined by photoemission measurements on an unpinned hydrogen terminated Si(111) surface[40, 41]. The vertical axis runs from 0 to 1.12 eV, the room temperature Si band gap. The solid diagonal line spanning the band gap shows the variation of the ideal Schottky-Mott barrier on silicon. The predictions of the screened defect pinning model for pinning at the divacancy levels, the interstitial and vacancy cluster ensemble levels, and the charge neutrality level, ϕ^*, are shown. The slope of these lines is determined entirely by the permittivity of Si and the assumption that the silicide

permittivity is infinite. The Schottky barrier height coincides with the defect level energy where the pinning model prediction intersects the Schottky-Mott prediction. Table I lists the silicides for which barrier heights are plotted in Figure 1, the silicide work function, and the references from which the barrier height data for each silicide was taken. The silicide work functions were computed according to the average charge transfer model described in Reference [12].

The data in Figure 1 can be separated into two groups. The first group contains only the rare earth silicides (*re*Si) which have work functions less than 4.0 eV and pin at defect levels in the upper half of the band gap. The second group consists of transition metal silicides (*tm*Si) which have work functions greater than 4.1 eV. The silicides with $\phi_{mSi} < 4.5$ eV have barriers determined by vacancy related defects. Those with $\phi_{mSi} > 4.5$ eV pin near the interstitial cluster level at $E_v + 0.48$ eV. For the *re*Si contacts the silicide work function is above the divacancy level in the absence of interfacial charge transfer. The divacancy is an acceptor and charge flows from the silicide into the divacancy. With screening the final barrier height for pinning exclusively to a V_2 level is slightly less than 0.4 eV. Vacancy clusters are known to give rise to a deep level transient spectroscopy (DLTS) peaks at E_c - 0.47 eV and E_c - 0.55 eV. Under appropriate processing conditions peaks the formation of V_n appears to be enhanced as demonstrated by the data for $GdSi_2$, most of the open square symbols just below the Si conduction band edge. That V_n clusters are also acceptors is consistent to the data points falling above the Schottky-Mott line. The behavior of $ErSi_{1.7}$, the mostly triangular symbols just above the Si conduction band edge, is qualitatively different. These contacts tend to favor the filling of states above the divacancy level. The one solid triangle with $\phi_{bn} = 0.29$ eV just below the conduction band edge is for what is

nominally $ErSi_2$. Er does not typically form a thin film disilicide on Si and this data point probably does correspond to the lower work function $ErSi_{1.7}$. Aside from noting that there are several acceptor type defects in the upper third of the Si band gap no attempt will be made identify those levels between the conduction band edge and the divacancy level. There is insufficient data to make a convincing assignment.

The lowest work function *tm*Si is HfSi with $\phi_{mSi} = 4.2$ eV. This is the only *tm*Si with published Schottky barrier data which has a work function above the V_2 level. It is also the only *tm*Si which pins to the V_2 level for appropriate processing conditions. For the three data points for (111) p-type contacts (open triangles) the effective n-type barriers increase monotonically with decreasing silicidation anneal temperature. For $GdSi_2$ contacts the barrier height was found to depend on the anneal time, anneal temperature and the thickness of the metal deposited prior to reaction. Hf metal is unique in that it has the lowest work function of all of the transition metals with ϕ_m = 3.9 eV. This is coincident with the Si conduction band edge. There was an early reports of Hf/p-Si Schottky contacts with the barrier pinned at E_c - 0.22 eV [42]. This report generated considerable discussion and the result was ultimately attributed to oxygen contamination at the Hf/Si interface [43, 44]. The vacancy-oxygen pair defect introduces a bulk acceptor level at E_c - 0.17 eV and anneals out at about 325 °C [45]. The low Hf work function is above the V-O level prior to interface formation and charge may be readily transferred into this acceptor. Annealing to form the silicide apparently dissociates the V-O complex and favors the formation of V_2, V_n , or V_n-O_m pinning levels[46]. With increasing work function the next four silicides (MnSi, $HfSi_2$, $TiSi_2$, $ZrSi_2$) have work functions between the V_2 level and the deepest V_n level. Generally, these appear to pin to the V_n level at E_c - 0.55 eV as do the largest

barriers for $GdSi_2$ and HfSi. The largest Schottky barrier in this range, MnSi with ϕ_{bn} ~ 0.76 eV, is attributed to an impurity related (carbon ?) midgap defect level.

The remaining silicides have work functions very close to or below the level of the I_n cluster level. The I_n level has donor character and for these contacts the interfacial dipole is characteristic of charge transferring from the Si defect levels to the silicides. Pinning at this level dominates the behavior of the high work function silicides. The donor character is evident in Figure 1 as the Schottky barrier data is below the Schottky-Mott line. When the silicide work function becomes deeper than the divacancy donor level it too can pin the Schottky barrier height. The very highest work function silicides are PtSi and Pt_2Si for which ϕ_{mSi} is deeper than the Si valence band edge. As near the conduction band edge, crossing the valence band appears to affect the stability of interfacial defects. Pinning at the V_2 donor is evident for PtSi contacts although there is a tendency to pin higher in the gap for most of the data. There are two possible explanations for this behavior. First, there is a known secondary interstitial cluster level at E_v + 0.29 eV. Second, there is the possibility that pinning is at a vacancy cluster. The evolution of the donor state of vacancy clusters has not been studied and is suggested as a logical corollary to the evolution of acceptor vacancy cluster states in the upper half of the band gap. Both $GdSi_2$ and HfSi are process sensitive following vacancy related levels. Of the high work function *tm*Si's those pinning close to V_2 donor level show a greater process sensitivity than those pinning close to the I_n level.

While there are a multitude of point defects known to exist in silicon Schottky barrier pinning is dominated by divacancies, vacancy clusters and interstitial clusters. The preferred pinning level is determined by the relative

positions of the silicide work function, the silicon band edges and the silicon defect levels located in an absolute frame of reference. Pinning at acceptor type defects controls barrier heights in the upper half of the band gap while pinning at donor is the rule in the lower half of the gap. The ability of the model to separate behavior relative to band edges and defect levels is taken as evidence that the computation of the silicide work functions is correct. If it were not, the behaviors of $ErSi_{1.7}$, $GdSi_2$ and HfSi would not be explicable as the measured work functions are much larger than the calculated values.

The present model is also consistent with reported variation of the temperature dependence of Schottky barrier heights. Acceptor states in the upper band gap typically track the conduction band with temperature while the donor states typically track the valence band edge. $ErSi_{1.7}$ contacts pinned to the V_2 acceptor level are tied to the conduction band edge [47]. $CoSi_2$, $TiSi_2$, WSi_2 and Cu_3Si contacts tied to the I_n donor level are tied to the valence band edge. PtSi, pinning close to the V_2 level donor level, is also tied to the valence band edge [47, 48]. Theoretical considerations indicate that defect levels may have mixed parentage from both the conduction and valence bands and consequently have a temperature dependence less than that of the band gap. Laterally inhomogeneous contacts pinning at two, or more, different defect levels are also expected to have intermediate temperature dependencies as well [49].

Closely related to temperature dependence of a Schottky contact is its pressure dependence. Using the intrinsic stress of as-deposited metals, varied by deposition conditions, it can be shown that W, pinning at the I_n level, has a barrier height on p-type Si which is largely independent of stress in the system while the n-type barrier is strongly dependent on stress [50, 51]. The barrier height on n-type Si was observed to vary by a little over 0.05 eV as a

function of stress in the as-deposited W. Much of the scatter in the data presented in Figure 1 is attributed to intrinsic stress in the silicide/silicon contacts as a function of processing conditions. While the effect of intrinsic stress on sputter deposited metal Schottky contacts has been documented less work has been reported for silicide contacts. What is known is that strain in the as-deposited metal does have a small effect on the silicide formation reaction rate [52] and that the interfacial strain is nonuniform under a silicide contact with strong variation occurring near the edges [53-56]. For large area contacts the effect of strain would be largely invisible if it were uniform across the contact. "Patchy" Schottky contacts are typically assumed to have regions of different barrier heights which are homogeneous within each patch [57]. The origin of the distinct barriers occurring within each region has not been adequately explained. Within the present model distinct barrier height may arise from local variations in defect type, contamination level[58], or from local variation in interfacial strain. As device dimensions shrink, edge effects will play an increasingly important role in determining the effective barrier height of a Schottky contact [59].

Strain effects may also explain barrier height variations around dislocations as detected by ballistic electron emission microscopy (BEEM) [60]. Dislocations in thin $CoSi_2$ contacts to (111) and (100) Si have been studied by BEEM. Variation of the barrier height on the order of 0.06 eV is observed when scanning across dislocations on (100) Si but not on (111) Si. Given the spacial scale the barrier height variation the dislocation core on (100) Si would have to produce a defect level at least 0.3 eV above that present at the surrounding interface. Interfacial strain will introduce both hydrostatic and shear strains in the silicon. Hydrostatic strain affects both interfaces identically. Shear strain affects only the (100) surface and will lift the

degeneracy of the 6-fold degenerate X symmetry conduction band edge driving two minima up or down in energy and four in the opposite direction depending on the sign of the strain. In the vicinity of the dislocation the shear strain is relived and the minima which have been driven down relax upward in energy toward the strain free location. The magnitude and direction of the barrier height variation across dislocations at (100) interfaces is consistent with just this kind of strain relaxation phenomenon.

What this work has not covered is unannealed elemental contacts and epitaxial contacts. The deposition of pure metals often results in the formation of a thin reacted silicide layer at the interface. In some cases, such as Pd and Co, crystalline silicides are formed upon room temperature deposition of the metal on a clean Si surface [61, 62]. Description of a thin interfacial silicide in terms of the work function variation across the metal/silicide/silicon structure is problematic when the silicide is only a few atomic layers thick. Second the barrier height of an as deposited metal contact will be sensitive to the method of deposition as all methods are known to introduce defects in the silicon well away from the interface and to introduce variable amounts of strain into the deposited metal [51, 63-69]. In epitaxial where a crystalline silicide is grown by codeposition at an elevated temperature an atomically smooth interface with coherent registry of the two crystals may be obtained. In $NiSi_2$ A and B type contacts the long range coherency of the atomic structure of the interface can generate an intrinsic dipole on the order of a tenth of an eV [70-74]. The A type interface pins close to the I_n level. It is possible that the intrinsic dipole is simply superimposed on of the defect dipole at the B type interface and that it too pins at the I_n level.

Finally, the present paper takes the literature values for barrier heights and silicide compositions at face value. Barrier evolution in the silicidation

process can be influences by metal deposition induced damage. Several studies have been done to evaluate the damage introduced during sputter deposition. Vacancy related defects with concentrations which decay exponentially away from the metal/silicon surface are implicated. The type and extent of the damage represents variation in the "initial conditions" for the silicidation reaction. Different initial near surface defect profiles result in slightly different final barrier heights. Similar observations can be made for the effect of different surface cleaning treatments of the silicon prior to metal deposition. [29, 75-81]

Extraction of barrier heights is sensitive to the ideality of the contact and the sophistication of the analysis performed on the measured diode response. Nonidealities can arise from lateral inhomogeneities in the barrier height, due either to strain or local variations in defect type and density. Near surface dopant profiles may be modified with the formation of near surface p-n junctions or the simple compensation of dopants by low concentrations of deep levels which more than about a nm from the interface. When current-voltage characteristics are used to assess barrier heights the analysis is often made by assuming that there is a bias range where thermionic current dominates. The presence of other current conduction paths introduces error into the analysis, especially for small barrier heights. A substantial amount of the scatter in the data is certainly related to the complexity involved in extracting a barrier height from experimental data [57, 82-87].

CONCLUSIONS

This work has combined three essential concepts to demonstrate the dominance of defect pinning of the Schottky barrier height for silicide/silicon

contacts. The first is the use of the screened pinning model to correlate defect level pinning with variation in the silicide work function. The second is the use of silicide work functions as corrected by the average charge transfer model to represent the bulk Fermi level in the silicide relative to the vacuum level. The third is the assertion that interstitial and vacancy clusters (as small as V_2) are the defects to be associated with pinning the Schottky barrier height. This is consistent with contact formation by solid phase reaction of a metal/silicon couple. The model is also sensitive to the correct location of the silicon band edges relative to the vacuum level. This has been possible only recently with the characterization of hydrogen passivated silicon surfaces. With this model it is now possible to estimate the range and stability of specific silicide Schottky contacts to silicon as well as their temperature dependence. Low work function silicide pin to vacancy related defects in the upper half of the band gap. These silicide are prone to be process sensitive as V_2 and several V_n cluster are sufficiently stable to determine the barrier height. Vacancy levels are tied to the conduction band giving temperature independent barriers to n-type Si and temperature dependent barriers to p-type Si. High work function silicides pin to donor type defects in the lower half of the band gap. These defects are tied to the valence band giving rise to a reversal of the temperature dependencies of n- and p-type Si contacts. Most of these contact are relatively insensitivity to process history. The significant exceptions are Pt silicides which are postulated to tract donor type V_n defects close to the valence band edge. The conventional wisdom that silicide barrier heights are highly reproducible is supported only for silicide with work functions in the range 4.38 - 5.02 eV which pin to the I_n cluster level.

ACKNOWLEDGEMENTS

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

REFERENCES

[1] J. M. Andrews and J. C. Phillips, "Chemical bonding and structure of metal-semiconductor interfaces," *Physical Review Letters*, vol. 35, pp. 56-59, 1975.

[2] A. Kikuchi, "Correlation between Schottky-barrier height and the heat of formation of transition-metal silicides," *Journal of Applied Physics*, vol. 74, pp. 3270-3272, 1993.

[3] J. L. Freeouf, "Silicide Schottky barriers: An elemental description," *Solid State Communications*, vol. 33, pp. 1059-1061, 1980.

[4] S. Hara and I. Ohdomari, "Chemical trends in silicide electronic structure and Schottky-barrier heights of silicide-silicon interfaces," *Physical Review B*, vol. 38, pp. 7554-7557, 1988.

[5] P. E. Schmid, "Silicide-silicon Schottky barriers," *Helvetica Physica Acta*, vol. 58, pp. 371-382, 1985.

[6] W. Mönch, "Metal-semiconductor contacts: electronic properties," *Surface Science*, vol. 299/300, pp. 928-944, 1994.

[7] W. Walukiewicz, "Fermi level dependent native defect formation: Consequences for metal-semiconductor and semiconductor-semiconductor interfaces," *Journal of Vacuum Science and Technology B*, vol. 6, pp. 1257-1262, 1988.

[8] R. J. Iwanowski, "Uniform mechanism of Fermi-level pinning at the Si-metal interface and in bulk silicon - phenomenological model," *Applied Surface Science*, vol. 56-58, pp. 348-355, 1992.

[9] A. Kikuchi, "Silicide-silicon Schottky barrier heights calculated using an interface-defect model," *Japanese Journal of Applied Physics*, vol. 37, pp. 2430-2432, 1998.

[10] T. J. Drummond, "Schottky barriers on GaAs: Screened pinning at defect levels," *Physical Review B*, vol. 59, 1999.

[11] S. P. Murarka, "Refractory silicides for integrated circuits," *Journal of Vacuum Science and Technology*, vol. 17, pp. 775-792, 1980.

[12] T. J. Drummond, "Work functions of the transition metals and metal silicides," *Journal of Applied Physics*, vol. to be submitted., 1999.

[13] I. D. Konozenko, A. K. Semenyuk, and V. I. Khivrich, "Radiation defects in Si of high purity," in *Radiation Effects in Semiconductors*, J. W. Corbett and G. D. Watkins, Eds. London, U. K.: Gordon and Breach, 1971, pp. 249-255.

[14] R. C. Young and J. C. Corelli, "Photoconductivity studies of radiation-induced defects in silicon," *Physical Review B*, vol. 5, pp. 1455-1467, 1972.

[15] J. W. Corbett, R. L. Kleinhenz, E. Wu, and Z. You, "Electron paramagnetic resonance studies in neutron-irradiated silicon," *Journal of Nuclear Materials*, vol. 108 & 109, pp. 617-626, 1982.

[16] J. W. Farmer and J. M. Meese, "Deep level transient spectroscopy of neutron irradiated semiconductors," *Journal of Nuclear Materials*, vol. 108 & 109, pp. 700-708, 1982.

[17] H. N. Yousif, D. L. Cowan, and J. M. Meese, "Cluster center formation in neutron-damaged silicon," *Journal of Applied Physics*, vol. 55, pp. 1359-1363, 1984.

[18] J. H. Svensson, B. G. Svensson, and B. Monemar, "Infrared absorption studies of the divacancy in silicon: New properties of the singly negative charge state," *Physical Review B*, vol. 38, pp. 4192-4197, 1988.

[19] A. Sienkiewicz and R. Iwanowski, "Four-vacancy damage clusters in neutron-irradiated silicon," *Materials Science and Engineering B*, vol. 4, pp. 247-250, 1989.

[20] M. W. Hüppi, "Proton irradiation of silicon: Complete electrical characterization of the induced recombination centers," *Journal of Applied Physics*, vol. 68, pp. 2702-2707, 1990.

[21] B. G. Svensson, B. Mohadjeri, A. Hallén, J. H. Svensson, and J. W. Corbett, "Divacancy acceptor levels in ion-irradiated silicon," *Physical Review B*, vol. 43, pp. 2292-2298, 1991.

[22] K. A. Abdullin, B. N. Mukashev, M. F. Tamendarov, and T. B. Tashenov, "Electronic levels and properties of the selfinterstitials in irradiated silicon," *Physics Letters A*, vol. 166, pp. 40-42, 1992.

[23] S. Dannefaer, P. Mascher, and D. Kerr, "Annealing studies of vacancies in proton irradiated silicon," *Journal of Applied Physics*, vol. 73, pp. 3740-3743, 1993.

[24] M. Asghar, M. Z. Iqbal, and N. Zafar, "Characterization of deep levels introduced by alpha radiation in *n*-type silicon," *Journal of Applied Physics*, vol. 73, pp. 3698-3708, 1993.

[25] Y. H. Lee, "Silicon di-interstitial in ion-implanted silicon," *Applied Physics Letters*, vol. 73, pp. 1119-1121, 1998.

[26] B. N. Mukashev, K. A. Abdullin, and Y. V. Gorelkinskii, "Self-interstitials in silicon irradiated with light ions," *physica status solidi (a)*, vol. 168, pp. 73-85, 1998.

[27] H. Kaupinnen, C. Corbel, J. Nissilä, K. Saarinen, and P. Hautojärvi, "Photoionization of the silicon divacancy studied by positron-annihilation spectroscopy," *Physical Review B*, vol. 57, pp. 12911-12922, 1998.

[28] J. Lalita, B. G. Svensson, and C. Jagadish, "Point defects observed in crystalline silicon implanted by MeV Si ions at elevated temperatures," *Nuclear Instruments and Methods in Physics Research B*, vol. 96, pp. 210-214, 1995.

[29] F. D. Auret, O. Paz, and N. A. Bojarczuk, "Characterization of ion-beam-sputtered molybdenum films on n-type silicon," *Thin Solid Films*, vol. 104, pp. 339-349, 1983.

[30] F. D. Auret, P. N. K. Deenapanray, S. A. Goodman, W. E. Meyer, and G. Myburg, "A deep level transient spectroscopy characterization of defects induced in epitaxially grown *n*-Si by low-energy He ion bombardment," *Journal of Applied Physics*, vol. 83, pp. 5576-5578, 1998.

[31] P. N. K. Deenapanray, F. D. Auret, M. C. Ridgway, S. A. Goodman, G. Myburg, and J. B. Malherbe, "Deep level transient spectroscopy characterization of 1 keV He, Ne, and Ar ion bombarded, epitaxially grown *n*-Si," *Journal of Applied Physics*, vol. 84, pp. 2565-2570, 1998.

[32] J. L. Benton, S. Libertino, P. Kringhøj, D. Eaglesham, J. M. Poate, and S. Coffa, "Evolution from point to extended defects in ion implanted silicon," *Journal of Applied Physics*, vol. 82, pp. 120-125, 1997.

[33] J. L. Benton, K. Halliburton, S. Libertino, D. J. Eaglesham, and S. Coffa, "Electrical signatures and thermal stability of interstitial clusters in ion implanted Si," *Journal of Applied Physics*, vol. 1998, pp. 9, 1998.

[34] W. Mönch, "Chemical trends of barrier heights in metal-semiconductor contacts: on the theory of the slope parameter," *Applied Surface Science*, vol. 92, pp. 367-371, 1996.

[35] T. J. Drummond, "Correlation between the atomic and bulk chemical potentials of low work function metals," *Journal of Applied Physics*, vol. 0, pp. 0, 1999.

[36] L. Fedina, A. Gutakovskii, A. Aseev, V. Landuyt, and J. Vanhellemont, "Extended defects formation in Si crystals by clustering of intrinsic point defects studied by in-situ electron irradiation in an HREM," *physica status solidi (a)*, vol. 171, pp. 147-157, 1999.

[37] A. La Magna, S. Coffa, and L. Colombo, "Role of extended vacancy-vacancy interaction on the ripening of voids in silicon," *Physical Review Letters*, vol. 82, pp. 1720-1723, 1999.

[38] S. Bensalah, J.-P. Lacharme, and C. A. Sébenne, "Effect of vacuum annealings on the electronic properties of clean Si(111) surfaces," *Physical Review B*, vol. 43, pp. 14441-14446, 1991.

[39] J. Dabrowski, H.-J. Müssig, and G. Wolff, "A novel surface reconstruction: subsurface interstitials stabilize Si(113)3×2," *Surface Science*, vol. 331-333, pp. 1022-1027, 1995.

[40] N. Safta, J.-P. Lacharme, C. A. Sébenne, and A. Akremi, "The influence of surface scattering on photoemission yield spectra in Si(111): consequences for ionization energy determination," *Journal of Physics: Condensed Matter*, vol. 5, pp. 6623-6630, 1993.

[41] V. Y. Aristov, G. Le Lay, K. Hricovini, A. Taleb-Ibrahimi, P. Dumas, R. Gunther, J. Osvald, and G. Indlekofer, "Nearly complete tuning of the Fermi level position at a prototypical metal-silicon interface: lead on unpinned Si(111)1x1-H," *Journal of Electron Spectroscopy and Related Phenomena*, vol. 68, pp. 419-426, 1994.

[42] A. N. Saxena, J. J. Grob, M. Hage-Ali, P. Siffert, and I. V. Mitchell, "Halfnium-silicon surface barriers," presented at Metal-semiconductor contacts, Manchester, U. K., 1974.

[43] C. R. Crowell, "A simplified self-consistent model for image force and interface charge in Schottky barriers," *Journal of Vacuum Science and Technology*, vol. 11, pp. 951-957, 1974.

[44] M. A. Taubenblatt, D. Thomson, and C. R. Helms, "Interface effects in titanium and hafnium Schottky barriers on silicon," *Applied Physics Letters*, vol. 44, pp. 895-897, 1984.

[45] G. D. Watkins, "Native defects and their interactions with impurities in silicon," presented at Defects and Diffusion in Silicon Processing, San Francisco, California, U. S. A., 1997.

[46] A. Kawasuso, M. Hasegawa, M. Suezawa, S. Yamaguchi, and K. Sumino, "An annealing study of defects induced by electron irradiation of Czochralski-grown Si using a positron lifetime technique," *Applied Surface Science*, vol. 85, pp. 280-286, 1995.

[47] J. Y. Duboz, P. A. Badoz, F. A. d'Avitaya, and E. Rosencher, "Evidence for Fermi-energy pinning relative to either valence band or conduction band in Schottky barriers," *Physical Review B*, vol. 40, pp. 15, 1989.

[48] M. O. Aboelfotoh, "On Schottky barrier inhomogeneities at silicide/silicon interfaces," *Journal of Applied Physics*, vol. 69, pp. 3351-3353, 1991.

[49] J. H. Werner and H. H. Güttler, "Temperature dependence of Schottky barrier heights on silicon," *Journal of Applied Physics*, vol. 73, pp. 1315-1319, 1993.

[50] M. Mamor, E. Finkman, and F. Meyer, "W/Si Schottky diodes: Effect of metal deposition conditions on the barrier height," presented at Thin Films: Stresses and Mechanical Properties V, Boston, Massachusetts, U. S. A., 1994.

[51] M. Mamor, E. Dufour-Gergam, L. Finkman, G. Tremblay, F. Meyer, and K. Bouziane, "W/Si Schottky diodes: effect of sputtering deposition conditions on the barrier height," *Applied Surface Science*, vol. 91, pp. 342-346, 1995.

[52] M. von Allmen, S. S. Lau, and M.-A. Nicolet, "The influence of stress on silicon thin film reactions: silicide formation," presented at Thin Film Interfaces and Interactions, 1980.

[53] Y. Wakayama and S. Tanaka, "Strain distribution around a $NiSi_2$/Si interface measured by convergent beam electron diffraction," *Applied Surface Science*, vol. 117/118, pp. 285-288, 1997.

[54] Y. Wakayama and S. Tanaka, "Strain effect on electronic states of Si near a Si/$NiSi_2$ interface measured by electron nanoprobe techniques," *Japanese Journal of Applied Physics*, vol. 37, pp. 408-413, 1998.

[55] I. De Wolf, D. J. Howard, K. Maex, and H. E. Maes, "Phase and mechanical stress in and surrounding $TiSi_2$ and $CoSi_2$ lines studied by micro-Raman spectroscopy," presented at Advanced Metallization for Future ULSI, San Francisco, California, U. S. A., 1996.

[56] B. B. Li, F. Huang, S.-L. Zhang, Y. Gao, and L. Zhang, "Micro-Raman spectroscopic study of two-dimensional stress distribution in poly-Si induced by $CoSi_2$ patterns," *Semiconductor Science and Technology*, vol. 13, pp. 634-636, 1998.

[57] R. T. Tung, "Electron transport at metal-semiconductor interfaces: General theory," *Physical Review B*, vol. 45, pp. 13509-13523, 1992.

[58] C. Detavernier, R. L. Van Meirhaeghe, R. Donaton, K. Maex, and F. Cardon, "Ballistic electron emission microscopy study of barrier height inhomogeneities introduced in Au/*n*-Si Schottky contacts by a HF pretreatment," *Journal of Applied Physics*, vol. 84, pp. 3226-3231, 1998.

[59] N. Chen, Y. Wang, H. He, and L. Lin, "Effects of point defects on lattice parameters of semiconductors," *Physical Review B*, vol. 54, pp. 8516-8521, 1996.

[60] H. Sirringhaus, T. Meyer, E. Y. Lee, and H. von Känel, "Spatial variations of hot-carrier transmission across $CoSi_2$/Si interfaces on a nanometer scale," *Physical Review B*, vol. 53, pp. 15944-15950, 1996.

[61] P. S. Ho, T. Y. Tan, J. E. Lewis, and G. W. Rubloff, "Chemical and structural properties of the Pd/Si interface during the initial stages of silicide formation," *Journal of Vacuum Science and Technology*, vol. 16, pp. 1120-1124, 1979.

[62] J. Y. Veuillen, J. Derrien, P. A. Badoz, E. Rosencher, and C. d'Anterroches, "Co/Si(111) interface: Formation of an initial $CoSi_2$ phase at room temperature," *Applied Physics Letters*, vol. 51, pp. 1448-1450, 1987.

[63] F. D. Auret and P. M. Mooney, "Deep levels introduced during electron-beam deposition of metals on *n*-type silicon," *Journal of Applied Physics*, vol. 55, pp. 988-993, 1984.

[64] F. D. Auret and P. M. Mooney, "Transient capacitance study of defects introduced by electron-beam deposition of metals on *p*-type silicon," *Journal of Applied Physics*, vol. 55, pp. 984, 1984.

[65] F. D. Auret, O. Paz, and N. A. Bojarczuk, "Characterization of process-induced defects and device properties of ion beam sputter-deposited Mo contacts on Si," *Journal of Applied Physics*, vol. 55, pp. 1581-1589, 1984.

[66] A. S. Vercaemst, R. L. Van Meirhaeghe, W. H. Laflère, F. Cardon, W. De Bosscher, and R. J. Schreutelkamp, "On the influence of sputter etch cleaning on the silicidation, the thermal stability and the electrical characteristics of Ti/*p*-Si contacts," *Solid-State Electronics*, vol. 36, pp. 753-759, 1993.

[67] A. L. De Laere, R. L. Van Meirhaeghe, W. H. Laflère, and F. Cardon, "On the influence of the surface pretreatment of a Si substrate on cobalt silicide formation," *Semiconductor Science and Technology*, vol. 5, pp. 745-751, 1990.

[68] H. L. Meyerheim, U. Döbler, and A. Puschmann, "Preparation-dependent Co/Si(100) (2×1) interface growth: Spontaneous silicide formation versus interstitial-site mechanisms," *Physical Review B*, vol. 44, pp. 5738-5744, 1991.

[69] J.-R. Chen and C.-H. Ho, "Temperature effects on internal stress in molybdenum thin films on single-crystal silicon," *Thin Solid Films*, vol. 104, pp. 251-255, 1983.

[70] R. T. Tung, "Schottky-barrier formation at single-crystal metal-semiconductor interfaces," *Physical Review Letters*, vol. 52, pp. 461-464, 1984.

[71] A. Chantre, A. F. J. Levi, R. T. Tung, W. C. Dautremont-Smith, and M. Anzlowar, "States at epitaxial $NiSi_2$/Si heterojunctions studied by deep-level transient spectroscopy and hydrogenation," *Physical Review B*, vol. 34, pp. 4415-4418, 1986.

[72] A. F. J. Levi, R. T. Tung, J. L. Batstone, J. M. Gibson, M. Anzlowar, and A. Chantre, "Electron transport through epitaxial metal/semiconductor heterostructures," presented at Interfaces, Superlattices, and Thin Films, Boston, Massachusetts, USA, 1986.

[73] J.-J. Yeh, "Stacking fault induced relative dipole at type *A/B* $NiSi_2/Si(111)$ interfaces and its correlation to the Si(111) 7×7 subunit cell structure," *Applied Physics Letters*, vol. 55, pp. 1241-1243, 1989.

[74] J. A. Kubby and W. J. Greene, "Comparison of the geometric structure and electron reflectivity of *A/B*-$NiSi_2/Si(111)$ and *U/F*-Si-7×7 interfaces," *Journal of Vacuum Science and Technology B*, vol. 10, pp. 1908-1913, 1992.

[75] F. H. Mullins and A. Brunnschweiler, "The effects of sputtering damage on the characteristics of molybdenum-silicon Schottky barrier diodes," *Solid-State Electronics*, vol. 19, pp. 47-50, 1976.

[76] L. P. Andersson and A. O. Evwaraye, "Electrical characteristics of sputtering-induced defects in n-type silicon," *Vacuum*, vol. 28, pp. 5-7, 1977.

[77] E. Grusell, S. Berg, and L. P. Andersson, "Electrical defects in silicon introduced by sputtering and sputter-etching," *Journal of the Electrochemical Society*, vol. 127, pp. 1573-1576, 1980.

[78] L. Quattropani, K. Solt, P. Niedermann, I. Maggio-Aprile, Ø. Fischer, and T. Pavelka, "Ballistic electron emission microscopy of Schottky diodes on RF-plasma-treated silicon," *Applied Surface Science*, vol. 70/71, pp. 391-395, 1993.

[79] F. D. Auret, M. Nel, and N. A. Bojarczuk, "Characterization of defects introduced during dc magnetron sputter deposition of Ti-W on *n*-Si," *Journal of Vacuum Science and Technology B*, vol. 4, pp. 1168-1174, 1986.

[80] O. O. Awadelkarim, P. I. Mikulan, T. Gu, K. A. Reinhardt, and Y. D. Chan, "Electrical properties of contact etched p-Si: A comparison between magnetically enhanced and conventional reactive ion etching," *Journal of Applied Physics*, vol. 76, pp. 2270-2278, 1994.

[81] P. N. K. Deenapanray, F. D. Auret, and G. Myburg, "Electrical characterization and annealing behavior of defect introduced in Si during

sputter etching in an Ar plasma," *Journal of Vacuum Science and Technology B*, vol. 16, pp. 1873-1880, 1998.

[82] V. Aubrey and F. Meyer, "Schottky diodes with high series resistance: Limitations of forward *I-V* methods," *Journal of Applied Physics*, vol. 76, pp. 7973-7984, 1994.

[83] J. H. Werner, "Schottky barrier and pn-junction *I/V* plots - small signal evaluation," *Applied Physics A*, vol. 47, pp. 291-300, 1988.

[84] D. Donoval, M. Barus, and M. Zdimal, "Analysis of *I-V* measurements on PtSi-Si Schottky structures in a wide temperature range," *Solid-State Electronics*, vol. 34, pp. 1365-1373, 1991.

[85] D. Donoval, V. Drobny, and M. Luza, "A contribution to the analysis of the *I-V* characteristics of Schottky structures," *Solid-State Electronics*, vol. 42, pp. 235-241, 1998.

[86] Y. Zhu, Y. Ishimaru, N. Takahashi, and M. Shimizu, "Correlation between current-voltage and capacitance-voltage characteristics of Schottky barriers diodes," *IEEE Transactions on Electron Devices*, vol. 45, pp. 2032-202036, 1998.

[87] G. Gomila and J. M. Rubí, "Relation for the nonequilibrium population of the interface states: Effects on the bias dependence of the ideality factor," *Journal of Applied Physics*, vol. 81, pp. 2674-2681, 1997.

[88] K. N. Tu, R. D. Thompson, and B. Y. Tsaur, "Low Schottky barrier of rare-earth silicide on *n*-Si," *Applied Physics Letters*, vol. 38, pp. 626-628, 1981.

[89] R. Nipoti, J. Garrido, and S. Guerri, "Samarium as a Schottky barrier on *p*-type-silicon," *Solid-State Electronics*, vol. 29, pp. 1267-1270, 1986.

[90] G. Eftekhari, "Rapid thermal annealing of W-Sm bilayers on p-type silicon," *Thin Solid Films*, vol. 199, pp. 23-28, 1991.

[91] H. Norde, J. de Sousa Pires, F. d'Heurle, F. Pesavento, S. Petersson, and P. A. Tove, "The Schottky-barrier height of the contacts between some rare-earth metals (and silicides) and *p*-type silicon," *Applied Physics Letters*, vol. 38, pp. 865-867, 1981.

[92] P. Muret, T. T. A. Nguyen, N. Frangis, G. Van Tendeloo, and J. Van Landuyt, "Photoelectric and electrical responses of several erbium silicide/silicon interfaces," *Applied Surface Science*, vol. 102, pp. 173-177, 1996.

[93] P. Muret, T. T. A. Nguyen, N. Frangis, and J. Van Landuyt, "Unpinning of the Fermi level at erbium silicide/silicon interfaces," *Physical Review B*, vol. 56, pp. 9286-9289, 1997.

[94] J. Y. Duboz, P. A. Badoz, F. A. d'Avitaya, and E. Rosencher, "Temperature dependence of Schottky barrier height on Si: Experimental evidence for Fermi energy pinning relative to either valence or conduction band," *Journal of Electronic Materials*, vol. 19, pp. 101-104, 1990.

[95] Z. J. Horváth, G. Molnár, B. Kovács, G. Petö, M. Andrási, and B. Szentpáli, "Effect of crystallization on the electrical and interface characteristics of $GdSi_2$/p-Si Schottky junctions," *Journal of Crystal Growth*, vol. 126, pp. 163-167, 1993.

[96] P. Muret, D. Elguennouni, M. Missous, E. H. Rhoderick, R. Baptist, and A. Pellissier, "Influence of defects upon the forward bias admittance of metal-semiconductor interfaces," *Applied Surface Science*, vol. 56-58, pp. 341-347, 1992.

[97] F. M. d'Heurle, M. O. Aboelfotoh, F. Pesavento, and C. S. Petersson, "Schottky barriers of scandium and scandium monosilicide on silicon," *Applied Surface Science*, vol. 53, pp. 237-239, 1991.

[98] K. E. Sundström, S. Petersson, and P. A. Tove, "Studies of formation of silicides and their barrier heights to silicon," *physica status solidi (a)*, vol. 20, pp. 653-668, 1973.

[99] F. C. T. So, C.-D. Lien, and M.-A. Nicolet, "Formation and electrical properties of $HfSi_2$ grown thermally from evaporated Hf and Si films," *Journal of Vacuum Science and Technology A*, vol. 3, pp. 2284-2288, 1985.

[100] S. Zaima, T. Yamauchi, Y. Koide, and Y. Yasuda, "Study on determining factors of low contact resistivity in transition metal-silicon systems," *Applied Surface Science*, vol. 70/71, pp. 624-628, 1993.

[101] M. Aboelfotoh and K. N. Tu, "Schottky-barrier heights of Ti and $TiSi_2$ on *n*-type and *p*-type Si(100)," *Physical Review B*, vol. 34, pp. 2311-2318, 1986.

[102] S. Ogawa, T. Kouzaki, T. Yoshida, and R. Sinclair, "Interface microstructure of titanium thin-film/silicon single-crystal substrate correlated with electrical barrier heights," *Journal of Applied Physics*, vol. 70, pp. 827-832, 1991.

[103] J. M. Andrews and M. P. Lepselter, "Reverse current-voltage characteristics of metal-silicide Schottky diodes," *Solid-State Electronics*, vol. 13, pp. 1011-1023, 1970.

[104] M. P. Lepselter and J. M. Andrews, "Ohmic contacts to silicon," presented at Ohmic Contacts to Semiconductors, 1969.

[105] M. Eizenberg and K. N. Tu, "Formation and Schottky behavior of manganese silicides on *n*-type silicon," *Journal of Applied Physics*, vol. 53, pp. 6885-6890, 1982.

[106] R. Thompson, M. Eizenberg, and K. N. Tu, "Schottky contacts of Gd-Pt and Gd-V alloys on *n*-Si and *p*-Si," *Journal of Applied Physics*, vol. 52, pp. 6763-6768, 1981.

[107] V. F. Drobny, "Nearly ideal unguarded vanadium-silicide Schottky-barrier diodes," *IEEE Transactions on Electron Devices*, vol. 33, pp. 1294-1298, 1986.

[108] J. A. Roth and L. B. Roth, "Interface structure and electrical behavior of Nb/Si junctions," presented at Thin Film Interfaces and Interactions, 1980.

[109] U. Erlesand and M. Östling, "Properties of iron silicide contacts to n- and p-type silicon," *Physica Scripta*, vol. T54, pp. 300-304, 1994.

[110] M. O. Aboelfotoh, "Temperature dependence of the Schottky-barrier height of tungsten on *n*-type and *p*-type silicon," *Solid-State Electronics*, vol. 34, pp. 51-55, 1991.

[111] D. Donoval, C. M. Snowden, V. Nagl, J. Racko, and M. Barus, "Modeling of $CrSi_2$-Si and $MoSi_2$-Si Schottky barrier contacts," *IEEE Transactions on Electron Devices*, vol. 42, pp. 1187-1189, 1995.

[112] M. O. Aboelfotoh, A. Cros, B. G. Svensson, and K. N. Tu, "Schottky-barrier behavior of copper and copper silicide on *n*-type and *p*-type silicon," *Physical Review B*, vol. 41, pp. 9819-9827, 1990.

[113] G. J. van Gurp, "Cobalt silicide layers on Si. II. Schottky barrier height and contact resistivity," *Journal of Applied Physics*, vol. 46, pp. 4308-4311, 1975.

[114] N. J. Woods and S. Hall, "Self-aligned cobalt disilide/silicon Schottky barrier contacts: fabrication, materials and electrical characterization," *Semiconductor Science and Technology*, vol. 11, pp. 1103-1105, 1996.

[115] P. E. Schmid, P. S. Ho, H. Föll, and T. Y. Tan, "Effects of variations of silicide characteristics on the Schottky-barrier height of silicide-silicon interfaces," *Physical Review B*, vol. 28, pp. 4593-4601, 1983.

[116] V. W. L. Chin, J. W. V. Storey, and M. A. Green, "A note on current-voltage measurements of *n*-type and *p*-type Pd_2Si Schottky diodes," *Solid-State Electronics*, vol. 34, pp. 215-216, 1991.

[117] S. Chand and J. Kumar, "Current-voltage characterization of Pd_2Si based Schottky diodes on p-type (111) silicon and evaluation of their barrier heights," *Solid-State Electronics*, vol. 38, pp. 1103-1104, 1995.

[118] G. Ottaviani, K. N. Tu, and J. W. Mayer, "Barrier heights and silicide formation for Ni, Pd, and Pt on silicon," *Physical Review B*, vol. 24, pp. 3354-3359, 1981.

[119] M. Wittmer, "Current transport in high-barrier IrSi/Si Schottky diodes," *Physical Review B*, vol. 42, pp. 5249-5259, 1990.

[120] D. Wörle, H. Grünleitner, V. Demuth, C. Kumpf, H. P. Strunk, E. Burkel, and M. Schulz, "Amorphous and crystalline IrSi Schottky barriers on silicon," *Applied Physics A*, vol. 66, pp. 629-637, 1998.

[121] I. Ohdomari, T. S. Kuan, and K. N. Tu, "Microstructure and Schottky barrier height of iridium silicides formed on silicon," *Journal of Applied Physics*, vol. 50, pp. 7020-7029, 1979.

[122] C.-A. Chang, "PtSi contact metallurgy: Comparison of different annealing sequences, annealing time and ambients, and deposition of Pt," *Journal of Applied Physics*, vol. 59, pp. 3116-3121, 1986.

[123] P. W. Pellegrini, C. E. Ludington, and M. M. Weeks, "The dependence of Schottky barrier potential on substrate orientation in PtSi infrared diodes," *Journal of Applied Physics*, vol. 67, pp. 1417-1420, 1990.

[124] M. Wittmer, "Conduction mechanism in PtSi/Si Schottky diodes," *Physical Review B*, vol. 43, pp. 4385-4395, 1991.

[125] P. G. McCafferty, A. Sellai, P. Dawson, and H. Elabd, "Barrier characteristics of PtSi/*p*-Si Schottky diodes as determined from *I-V-T* measurements," *Solid-State Electronics*, vol. 39, pp. 5 83-592, 1996.

Silicide	ϕ_{mSi} (eV)	ϕ_{bn}/ϕ_{bp} references
$DySi_2$	3.76	[88]
$SmSi_{1.7}$	3.72	[89, 90]
$HoSi_2$	3.89	[88]
$ErSi_{1.7}$	3.85	[91-93]
$ErSi_2$	3.92	[47, 88, 94]
$GdSi_2$	3.93	[88, 95]
$YSi_{1.7}$	3.85	[91, 96]
YSi_2	3.93	[88]
ScSi	3.94	[97]
HfSi	4.20	[42, 98-100]
$HfSi_2$	4.33	[99, 100]
$TiSi_2$	4.36	[101, 102]
$ZrSi_2$	4.40	[103, 104]
MnSi	4.33	[98, 105]
VSi_2	4.51	[106, 107]
$NbSi_2$	4.51	[108]
FeSi	4.57	[109]
WSi_2	4.62	[110]
$MoSi_2$	4.64	[85, 111]
Cu_3Si	4.65	[112]
$CoSi_2$	4.76	[47, 113, 114]
RhSi	4.83	[103, 104]
Pd_2Si	4.98	[115-117]
Ni_2Si	5.00	[115, 118]

NiSi	4.92	[115]
$NiSi_2$	4.84	[115]
IrSi	5.00	[119, 120]
$IrSi_3$	4.84	[121]
Pt_2Si	5.17	[118]
PtSi	5.05	[118, 122-125]

TABLE I The table provides a list of the silicides for which Schottky barrier data has been collected and presented in Figure 1. The silicide work function and references to the Schottky barrier data for each silicide are given. No reliable citations were found for $TaSi_2$ (ϕ_{mSi} = 4.25 eV) which has a nominal characteristic barrier of ϕ_{bn} = 0.59 eV [1].

FIGURE CAPTIONS

Figure 1) Schottky barrier heights to n-type Si (ϕ_{bn}) are shown as solid triangles and squares for contacts to (111) and (100) Si surfaces, respectively. Schottky barriers to p-type silicon are shown as open symbols representing the equivalent n-type barrier computed as (E_g - ϕ_{bp}). The horizontal scale is the silicide work function which nominally locates the silicide work function relative to the vacuum level. The vertical dashed lines locate the Si conduction (3.90 eV) and valence band (5.02 eV)edges relative to the vacuum level. The vertical axis runs from 0 to 1.12 eV, the room temperature Si band gap. The solid diagonal line spanning the band gap shows the variation of the ideal Schottky-Mott barrier on silicon. The labeled solid line indicate the prediction of the screened pinning model for several defect levels.

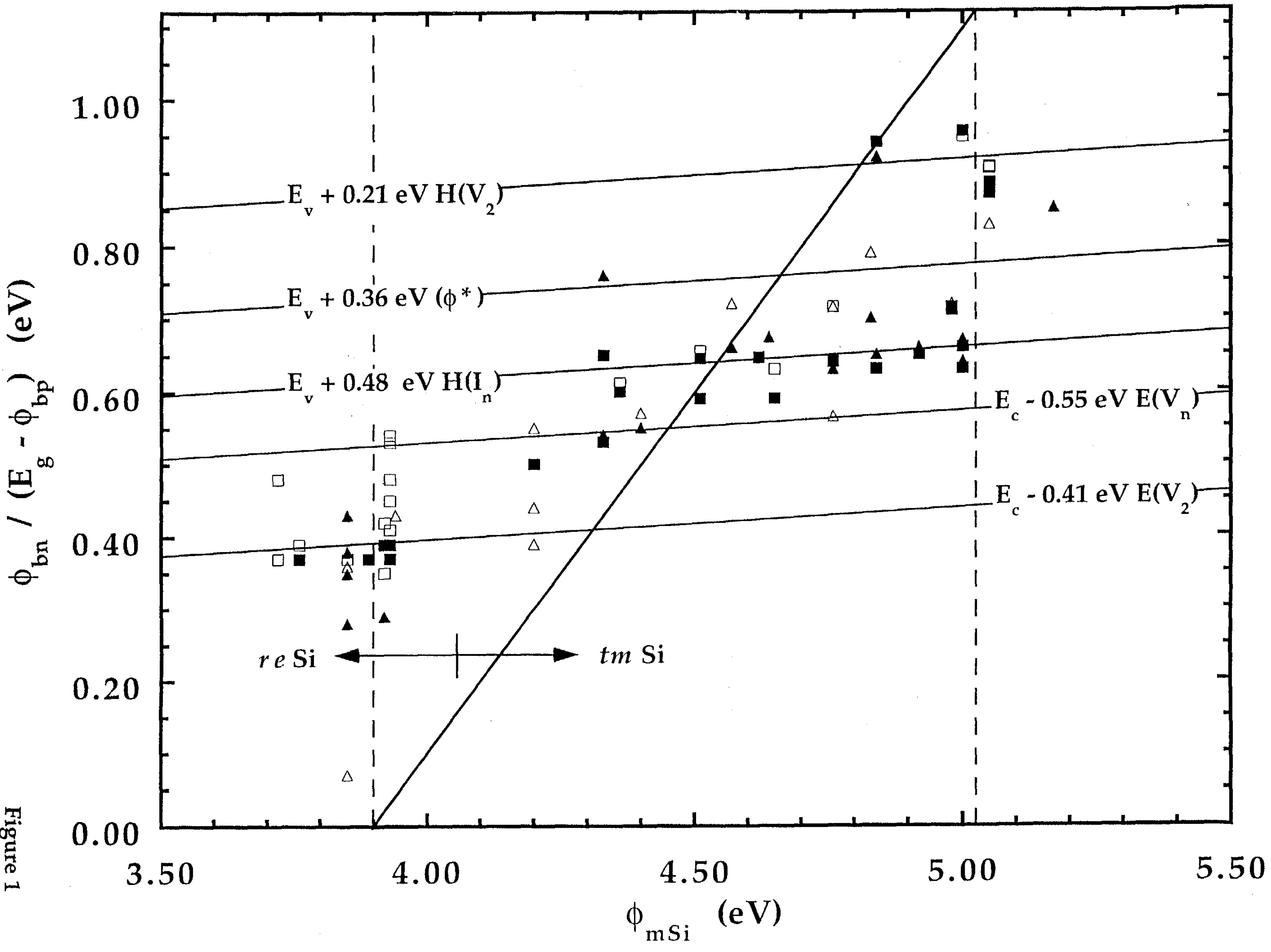

Figure 1