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Schottky Barrier Heights of Atomically-Controlled Silicide/Silicon Interfaces

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The Schottky barrier height (SBH) measured at epitaxial silicide/Si contacts is shown to be dictated by the silicide structure. The importance of controlling the structure of the epitaxial silicide interfaces by careful growth conditions is stressed. Structural inhomogeneity at the metal/semiconductor (MS) interface is shown to lead to spatial inhomogeneity in the SBH. In order to understand the formation mechanism of the SBH, it seems necessary to first understand the interfacial atomic structure at MS contacts.

I. INTRODUCTION

There have been extensive experimental and theoretical studies on the nature and formation of the Schottky barrier (SB) at MS interfaces.[1)] The importance of the interface atomic structure in influencing the electrical properties of MS contacts has often been overlooked, however, partly because of the lack of atomic level theories for Schottky transport and partly because of the difficulty in controlling and characterizing MS interface structures. Recently, it was shown that the Fermi level (FL) at most polycrystalline MS interfaces is not pinned at a unique energy defined by defect states[2)] or metal-induced gap states (MIGS),[3)] rather it fluctuates with significant amplitudes from region to region within one SB junction.[4-5)] When a MS interface has an inhomogeneous SBH, the SBH experimentally obtained from this interface is just an average value of some weighted distribution of different FL positions. Such an average does not necessarily carry any physical significance. Therefore, traditional approaches of comparing only the magnitudes of the experimental SBH's are likely fortuitous to reveal the formation mechanism of the SB! The true formation mechanism of the SB is obviously the one which decides locally the FL position from some specifics of the MS interface — which may be laterally varying. This local SB mechanism is most conveniently, and only explicitly, revealed in MS systems with homogeneous, well-characterized, interface structures. Single crystal epitaxial silicide/Si interfaces, because of their unsurpassed structural perfection among all MS junctions, have become the most ideal system to reveal the microscopic SB mechanism. In this presentation, the latest SBH results from epitaxial silicide/Si interfaces are described and their unmistakable implications are discussed.

II. SUMMARY OF RESULTS

The fabrication and the atomic structures of nearly perfect $NiSi_2$/Si(111) interfaces have been well documented.[6-7)] I-V measurements for the guarded $NiSi_2$/Si(111) diodes are shown in Fig. 1 for two substrate doping concentrations, high doping (HD) and low doping (LD) concentration. A ~ 140mV difference in SBH was consistently found between Type A and Type B $NiSi_2$ films, in agreement with earlier findings.[8-9)] SBH results are summarized in Table I. There was no difference found, within < 1%, between the I-V measurements on the thick or thin diodes. In addition, the presence or absence of dislocations in Type A films and a change in dislocation density in Type B films had no influence on the measured electrical properties. This contradicts the thickness-dependent SBH's observed for $NiSi_2$/Si(111) films observed by Kikuchi, et al.[10)] The dependence of the $NiSi_2$/Si(111) SBH on orientation has already been explained by theoretical calculations[11-12)] as arising from a difference in the interface atomic structure.

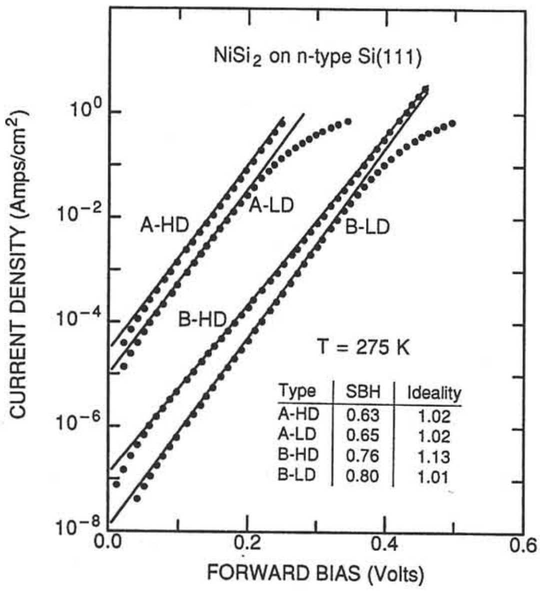

Fig. 1 I-V plots for diodes with $NiSi_2$ on n-type Si(111). Results from Type A (labeled A) and Type B (labeled B) diodes are shown for diodes on Si with higher doping concentration of 3.5×10^{16} cm^{-3} (HD) and a lower doping concentration of 6.3×10^{14} cm^{-3} (LD).

Table I. Summary of $NiSi_2$ SBHs

Film	Type	n-type SBH (V)
$NiSi_2(111)$	type A	0.65
$NiSi_2(111)$	type B	0.79
$NiSi_2(100)$	planar	0.40
$NiSi_2(100)$	all faceted	0.65

In contrast to Type A $NiSi_2$/Si(111), which may be grown free of any extended defects, $NiSi_2$ on Si(100) necessarily contains interfacial dislocations of Burgers vector a/4<111> at odd step height changes at the $NiSi_2$/Si(100) interface.[13] In addition, Ni-rich deposition and annealing at lower temperatures (< 600°C) invariably leads to the formation of "facet bars" bounded by {111} planes at the interface. The methods to control the layer morphology of thin $NiSi_2$ layers on Si(100) have been described in detail recently.[13] The n-type SBH of high quality, planar, $NiSi_2$/Si(100) interface is considerably lower than that of either of the $NiSi_2$/Si(111) interfaces.[14] The presence of facet bars has almost no effect on the n-type I-V characteristic of an otherwise uniform $NiSi_2$/Si(100) interface, but it has a very significant effect on the p-type characteristics (Fig. 2).[14] These observations and the non-idealities in the electrical properties of diodes containing facet bars may be readily explained on the basis of a spatial variation of the local SBH.[4-5,14]

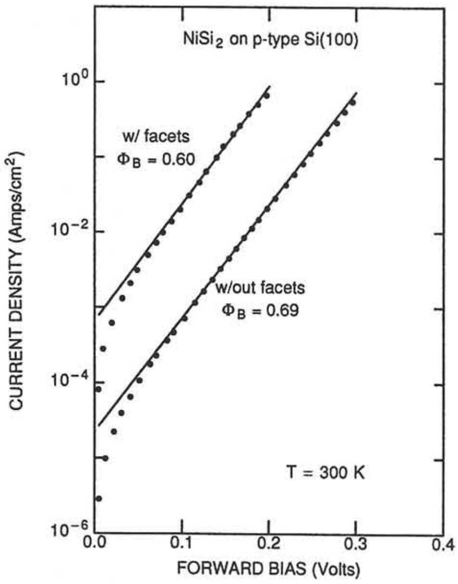

Fig. 2 I-V plots for partially faceted and planar $NiSi_2$ films on p-type Si(100).

III. CONCLUSIONS

We have shown that the SBH's of a number of high quality single crystal $NiSi_2$/Si interfaces are not determined by FL pinning. Rather, the interface dipole which determines the SBH seems to depend much on the atomic structure of the MS interface. This experimental finding may have more universal implications than presently realized. There is no evidence to suggest that the SBH at non-epitaxial MS interfaces would be determined by an entirely different mechanism. Indeed, the apparent lack of a strong dependence of the SBH on metal work function, usually construed as due to FL pinning, may simply be the result of SBH averaging. With the basic concepts of SBH formation firmly established by the present results, we are now in position to face more intriguing questions from more complex MS systems.

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