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LETTER TO THE EDITOR

Pressure dependence of the Schottky barrier height at the nickel-silicide/silicon interface

T-H Shen and C C Matthai
Department of Physics, University of Wales College of Cardiff, Cardiff CF1 3TH, UK

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Abstract. We have calculated the pressure coefficients of the silicon band gap and the Schottky barrier height at the $NiSi_2$/Si interface. The results are in very good agreement with experiment and suggest that this system is described by a metal-induced gap states model.

Schottky barriers at metal–semiconductor interfaces have attracted much attention over the past few decades. In recent years, one of the principal interests has centred on the mechanism for the pinning of the metal Fermi level in the band gap of the semiconductor. Among others, semiconductor surface states, metal induced gap states (MIGS),[1] defect levels in the gap and disorder induced gap states (DIGS) have all been thought to be responsible for Fermi level pinning. Dependent on the particular system, one of these mechanisms dominates. However, in most cases, it is not possible to identify the dominant mechanism. Pressure studies can be very helpful in differentiating between the possible mechanisms in some instances. For example, the energy dependence of defect levels with pressure would in general be different from the variation of the semiconductor and metal valence/conduction band energies. This would correspond to the pinning position varying with pressure. Shan *et al* (1988) measured the Schottky barrier height (SBH) of the Pt/GaAs interface as a function of pressure and found that its value shifted to higher energies with a linear pressure coefficient of 11 meV $kbar^{-1}$ and a non-linear coefficient of -0.26 meV $kbar^{-1}$. They concluded that these results were consistent with the amphoteric native defect model of Schottky barrier formation.

In addition to providing information about the validity of proposed models, pressure measurements offer a stringent test for the results of calculations. Because of its homogeneity and abruptness, the $NiSi_2$/Si (111) interface has been considered an ideal system for the comparison of theoretical predictions with experimental results. $NiSi_2$ grows epitaxially on Si (111) with its structure either in phase with that of the substrate (type A) or rotated by 180° with respect to the substrate (type B). The measured Schottky barier height for the two types was found to be different by 0.14 eV. There have been calculations based on the linear muffin-tin orbital (LMTO) and the tight-binding models which have claimed to explain this observed difference. A study by Rees and Matthai (1989) based on the linear combination of atomic orbital (LCAO) method in the extended Hückel approximation attributed the difference in the SBH to the different amounts of interface relaxation for the type A and type B systems, the most recent and exhaustive LMTO calculation by Ossicini *et al* (1990) arrived at the same conclusion. The argument

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Table 1. Calculation of the silicon band gap with pressure. a is the equilibrium lattice constant for Si. Δa is the change of the lattice constant under pressure. E_g^{expt} is the energy gap derived from the known experimental pressure coefficient (Welber *et al* 1975 (whilst E_g^{cal} is the calculated energy band gap.

$-\Delta a/a$ (%)	Equivalent pressure, P (GPa)	E_g^{cal} (eV)	E_g^{expt} (eV)	E_g^{expt}/E_g^{cal}
0.00	0.00	1.350	1.12	0.83
0.28	0.85	1.325	1.11	0.84
0.55	1.7	1.300	1.10	0.84
0.92	3.1	1.275	1.08	0.85
1.84	7.1	1.200	1.02	0.85
2.76	12.4	1.125	0.95	0.84

proposed by Rees and Matthai (1989) was that as the nickel silicide relaxes towards the substrate the SBH reduces and a relaxation of 0.1 Å resulted in a barrier height reduction of 0.15 eV. A further complication in these epitaxial systems is that experimental measurements of the interface bond lengths have given contradictory results. Only Zegenhagen *et al* (1989) have reported greater relaxation at the type A interface.

To examine the effect of changing bond length on the SBH, Werner (1989) performed measurements of the barrier heights for several silicide–silicon interfaces under hydrostatic pressure. From the results, it was concluded that the pressure coefficient of -0.8 meV kbar^{-1} for $NiSi_2$/Si was too small to explain the barrier difference of 140 meV based on the measured interface bond lengths. However, their conclusions were based on the assumption that there is a direct correlation between hydrostatic pressure and the interlayer bond length at the interface. Although the latter does indeed decrease with increased pressure, the $NiSi_2$ and Si bulk band structure are also modified.

In this letter, we report the results of calculations performed on the $NiSi_2$/Si type A and type B interfaces under hydrostatic pressure. We used the self-consistent LCAO method in the extended Hückel approximation to perform the calculations. As in the previous study, a supercell geometry consisting of eight layers of $NiSi_2$ and twelve layers of Si were used to model the interface structure. Self-consistency is incorporated by modifying the ionization potentials according to the amount of excess charge on each atom site. This is an essential feature, since one of the important contributions to the Fermi level pinning is the dipole at the interface. Once the self-consistent electronic structure and potential is calculated over the supercell, the local density of states across the unit cell is determined. From a knowledge of the separation of top of the valence band in the Si 'bulk-like' region from the Fermi level in the cell the SBH is computed. Hydrostatic pressure was simulated by reducing the lattice constant of the supercell. The calculations were performed for different lattice constants on both type A and type B interface structures. We have also considered the cases of interface bond relaxation in both structures. The change in SBH with lattice constant follows the same trend as that for the unrelaxed interfaces. In table 1 we list the pressure corresponding to the reduction in the lattice constant based on the non-linear bulk modulus (Nielsen 1987):

$$\Delta p = -98.8/(a/3\Delta a + 4.11)\ (\text{GPa}).$$

Also given are the calculated silicon band gaps. The pressure coefficient of the band gap

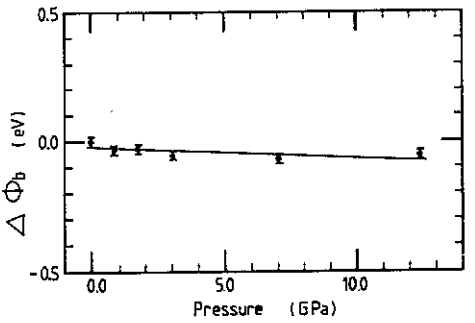

Figure 1. The calculated change of Schottky barrier height ($\Delta\Phi_b$) with pressure for type A unrelaxed $NiSi_2$/Si interface. From the slope of the fitted line, a pressure coefficient of -5 meV GPa^{-1} is obtained.

is found to be -18 meVGPa^{-1}, in very good agreement with the experimental value of -14 meV GPa^{-1} (Welber *et al* 1975). Because the calculated band gap is slightly higher than that determined from experiment, we have scaled the SBH, $\Phi_b = E_g - \Phi_0$, by the factor E_g^{expt}/E_g^{cal}, where Φ_0 is the difference between the Fermi level and the top of the 'bulk-like' Si valence band. As an example, the resulting changes of barrier height with pressure are plotted as a function of the equivalent pressure tabulated above for the type A interface (figure 1). Note that there is a large uncertainty in the determination of the Fermi level reflected in the large error bars on the SBH values. However, it can be clearly seen that there is a decrease in Φ_b with increasing pressure and this is much smaller than the difference with Φ_b for the type A and type B interfaces. We estimate the negative pressure coefficient of Φ_b to be 5 meV GPa^{-1} (0.5 meV kbar^{-1}), which is in very good agreement with experiment.

From the results of this work we may draw three main conclusions. The agreement of the pressure coefficients of the band gap and Φ_b with experiment indicates the usefulness of the empirical method in describing this system. Secondly, that our calculations, which are based on an abrupt interface with no defects, are able to account for the pressure dependence of Φ_b suggests that the nickel silicide/silicon interface is one where the MIGS model is favoured as the dominant Fermi level pinning mechanism. Finally, the difference between the type A and type B barrier heights are mainly due to an internal pressure resulting in a relaxation of the interface bond length. This local 'pressure' is expected to be much larger than the pressures we have considered in this letter.

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