Extended Abstracts of the 2017 International Conference on Solid State Devices and Materials, Sendai, 2017, pp715-716

PS-1-01

Schottky Barrier Heights of Metal Silicides on Si and Ge

J Robertson, H Li,

[1] Engineering Dept, Cambridge University, Cambridge CB2 1PZ, UK
Phone: +44-1223-748331 E-mail: jr@eng.cam.ac.uk

1. Introduction

Contact resistances limit the performances of highly scaled devices. These depend on the Schottky Barrier heights (SBHs) of the contact metals. The SBH φ tends to vary linearly with the work function of the metal Φ, with a rate S = dφ/dΦ. If this 'pinning factor' S is large, then the n-type or p-type SBH can be reduced to a small value by choosing the right metal. But often, for elemental metals on Si or Ge, S is very small [1] and this method fails. This is a particular problem for n-type Ge, where SBHs are pinned close to the valence band edge. However, it was found that silicides behave differently, having a much larger S value, fig 1 [2]. Thus small n-type SBHs can be achieved by using rare earth silicides, as rare earths have low work functions, and thus give small φn values. Recently Nishimura [3] found a similar behavior for germanides on Ge, and also that φn depends on crystal face. Here we extend and simplify our previous analysis of silicide SBHs to explain this.

2. Method

Here, we study Si/silicide interfaces, using the $NiSi_2$/Si structure to model large work function (small atomic rardius) metals, and the YSi_2/Si structure to model low work function (large atomic radius) metals. $NiSi_2$ has the fluorite structure and it is lattice-matched to Si. We take the A interface orientation, as in Fig 2(a).

In bulk $NiSi_2$, Ni sites are 8-fold coordinated by Si, and Si sites are 4-fold coordinated by Ni. At the Si:$NiSi_2$(111)A interface, the $NiSi_2$ lattice terminates as a 7-fold Ni site, which can be viewed as a Ni 'dangling bond', while the Si sites remain 4-fold bonded across the interface. The (100) interface has been much less studied. Its structure was proposed by Yu [4] and confirmed by Falke [5], Fig 2(b), and has a 2x1 reconstructed interface, with 5-fold Si sites and lateral Si-Si bonds on the Si side. The structure of the (110) interface is unknown, but a possible version is Fig 2(c).

YSi_2 has a hexagonal lattice and it is lattice-matched to the (111) face of Si, Fig 3(a). While YSi_2 is hexagonal, its *a* and *c* lattice constants are similar. A (100)Si/YSi_2 interface can be made by rotating the YSi_2 lattice, to give the structure shown in Fig 3(b).

The calculations are carried out on supercells of 5 layers of silicide and 9 layers of Si. The lattice geometry is relaxed in GGA. When there is no lattice-matching, the x,y lateral distances are fixed to those of Si, and the vertical z distances can relax. The local electronic structure is calculated, and the SBH energy is extracted as the energy from the Fermi level to the Si conduction band edge.

3. Results.

The φn values are plotted against the silicide work function in Fig 4. The silicide work function is estimated from the work function of the parent metal using a Miedema relation, WF = $(\Phi_M \Phi_{Si}^2)^{1/3}$. We see that the calculated φn values lie on separate lines for (100) and (111) faces, with continuity between data points for $NiSi_2$ and YSi_2 structures. The (100) data are offset upwards from the (111) data. The slopes are large, of order S~0.4, whereas those of elemental metals are very small (S~ 0.05) [1]. The increased slope is consistent with the experimental results [3], and supports the data. However the offset between (100) and (111) is in the opposite direction to that seen experimentally [3].

This shows that silicide SBHs are much less strongly pinned than the SBHs of elemental metals. This is valuable for obtaining small SBH values for n-type contacts for Ge.

4 Discussion

What is the cause of the different behavior of elemental metals and silicides? The silicides are metals but with covalent bonding between the metal and Si sites. The SBH of a defect-free metal-semiconductor junction is controlled by the pinning of the metal's Fermi level to the semiconductor's charge neutrality level (CNL). The CNL is the average energy of the metal induced gap state (MIGS) [4]. The MIGS are the evanescent states in the semiconductor gap which are extensions of the travelling wave states in the metal. They are composed of states drawn from the semiconductor's conduction and valence bands, and thus are intrinsic to the semiconductor itself [4]. They do not depend on the metal. Thus in the simple MIGS model, the SBH should not depend on the type of metal, if elemental or compound/ silicide.

The MIGS can be thought of as the dangling bonds of the free Si surface having been dispersed by contact with the metal into MIGS, Fig 5,6 [2]. So silicides are different from elemental metals in that their Si interfaces have DBs on the metal sites in the silicide, not on the silicon side, Fig 7. Thus whereas for an interface between Si and a normal metal, S is a function of the Si, but for a silicide interface, S is a function of the silicide and the metal with the DB on it. As this metal of the silicide changes, this enters into the equation for S, and S increases, see Fig 8.

References

1. T Nishimura, K Kita, A Toriumi, APL 91 123123 (2007)
2. L Lin, Y Guo, J Robertson, APL 101 052110 (2012)
3. T Nishimura, T Yajima, A Toriumi, App Phys Exp 9 081201

(2016); SSDM (2016) O-6-02.
4. J Tersoff, Phys Rev Lett 52 465 (1984); W Monch, Phys Rev Lett 58 1260 (1986)
5. B D Yu, et al, J Vac Sci Technol B 19 1180 (2001)
6. U Falke, et al, Phys Rev Lett 92 116103 (2004)

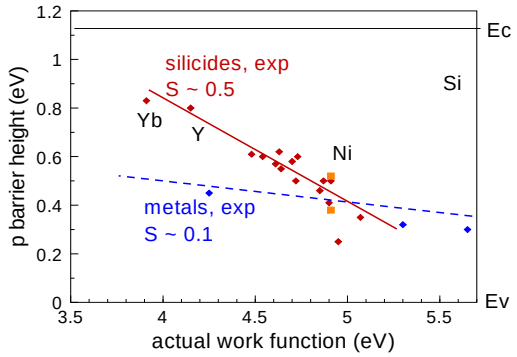

Fig. 1. Experimental SBHs for elemental metals and silicides on Si

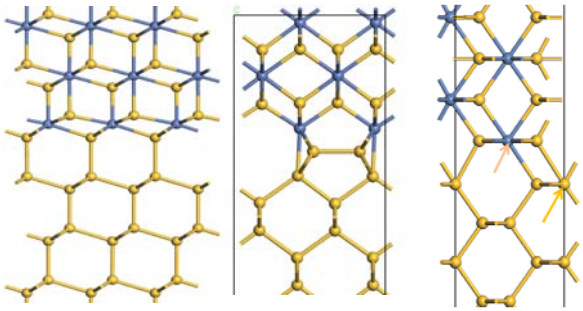

Fig. 2. (111), (100) and (110) structures for Si/ $NiSi_2$ interface.

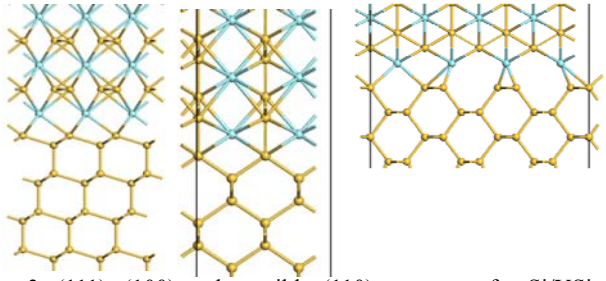

Fig. 3. (111), (100) and possible (110) structures for Si/YSi_2 interfaces

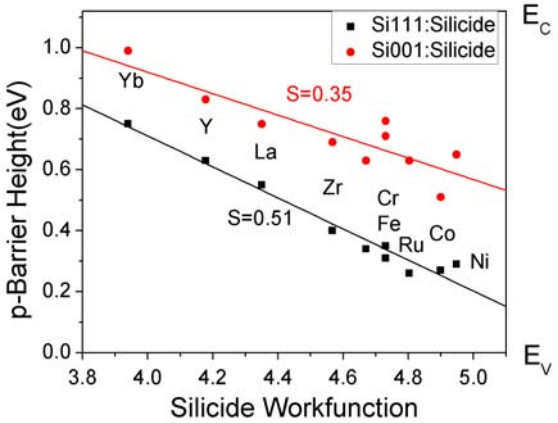

Fig. 4. Calculated Schottky barrier heights (SBHs) for (111) and (100) Si/MSi_2 interfaces

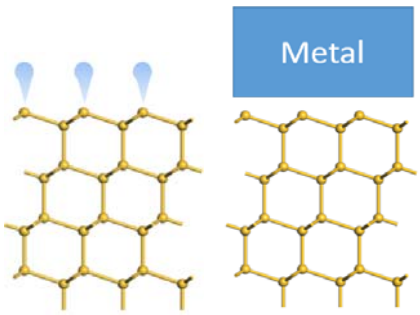

Fig. 5. Schematic of Si DBs converting into MIGS at metal-Si interface.

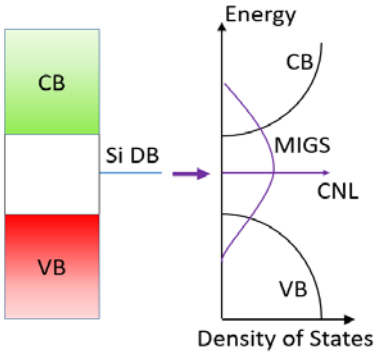

Fig. 6. Development of Si DB into MIGS and its average energy, the CNL.

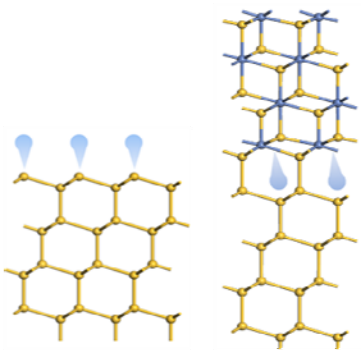

Fig. 7. The dangling bonds on a Si surface, and the Ni DBs at the Si/$NiSi_2$ interface.

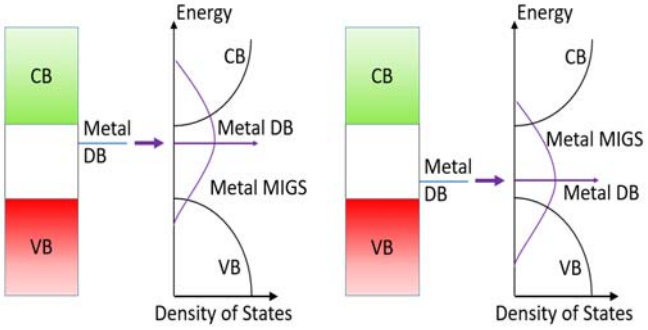

Fig. 8.How the metal dangling bonds and their resulting MIGS control the energy of the MIGS and CNL.