What determines Schottky Barrier Heights of Metal Silicides on Si and Ge

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Abstract

The standard MIGS model from Bardeen and Heine notes that the Si surface ends in a series of dangling bonds (DBs) whose states lie in the Si gap. When a metal is put on the Si, the plane wave states of the metal cause the DB states to spread out across its Penn gap, and these DBs become MIGS (Fig 4). The CNL is the average energy of the original DBs, lying at the DB energy [8]. Thus the SBH does not vary much with the metal work function.

Now, at a Si:NiSi$_2$ interface, the Si sublattice is continuous across the interface; there are no Si dangling bonds. The DBs are on Ni atoms on the silicide side. It is these states that spread across the interface and now create the MIGS (Fig 4b). Thus the MIGS and CNL can now depend on the silicide metal work function and interface geometry. This is exactly what happens at the A and B interfaces of (111)Si:NiSi$_2$. Thus, it is not an interface dipole effect, nor does it require replacing the MIGS model.

We now extend this idea to other silicides. Various rare earth silicides such as YSi$_2$ are lattice matched to Si. This has a hexagonal lattice with the metal sites forming planes and the silicon in a sandwich [12]. It has highly ionic bonding due to the very electropositive Y, as seen from its valence charge density (Fig 2b). The Si sublattice is again continuous across the (111)Si:YSi$_2$ interface. The highest filled state at the interface is a polar Y-Si bonding state, mainly localised on the last Si of the Si side (Fig 3c). The metal DB state is now much higher in the conduction band (Y is very electropositive), so the n-type SBH is much reduced. The experimental p-type SBH is 0.8 eV.

Thus, the SBH of silicides are not pinned to the same degree as at normal metal–Si SBs, because they change with the metal DB energy, and are not pinned at the Si CNL. The calculated SBHs given in Fig 1 show a strong dependence on metal work function, and would lie well above the Si CNL. Note that the calculated barriers lie below the experimental values because of the band gap error of the local density approximation. In addition, the interface geometry is seen to vary the SBH.

Fig 2d shows the case of (111)Si:Fe$_3$Si. Fe is slightly more electropositive than Ni, but the bonding is still relatively non-polar. The Si sublattice is continuous [2]. The highest occupied state is again a metal DB (Fig 3d).

References


Fig. 1. Experimental Schottky Barrier heights of silicides [4] and pure metals [6] on Si, plotted against (a) actual work function and (b) work function of parent metal, compared to silicide SBHs calculated by LDA. Note that LDA points lie lower in the gap than experimental values due to LDA band gap error.

Fig. 2(a) Valence charge density of Si:NiSi2, with a non-polar spread between Ni and Si sites. Large charge density near Ni is the 3d electrons.

(b) Valence charge density of Si:YSi2, with valence charge localised near Si in the silicide.

Fig. 3. Highest occupied state for (a) NiSi2 A, (b) NiSi2 B, (c) YSi2, (d) Fe3Si.

Fig. 4(a). How surface Si dangling bonds develop into MIGS on a metal covered surface. (b) For a silicide interface, all Si DBs are bonded to metal atoms, leaving metal DBs to form the interface states. Metal DB energies vary with metal work function, unlike a CNL.