

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

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1. Introduction

The large contact resistances and large Schottky Barrier heights (SBHs) of n-type Ge can be mitigated by using silicide contacts such as (111)Ge:Fe₃Si [1,2]. Rare earth silicides are another popular way to reduced n-type barrier heights [3]. The slope of barrier height vs. metal work function is higher for silicides [4,5] than for pure metals [6], indicating weaker Fermi level pinning in silicides (Fig 1). However, the reason is not known. We show here that this arises from the different interface bonding.

The SBH of a metal-semiconductor junction should be controlled by the pinning of the metal Fermi level to a semiconductor reference energy which in the metal induced gap state (MIGS) model is the charge neutrality level (CNL)[7]. To this SBH can be added a voltage offset due to any interface dipoles. But a fundamental point is that, in the well screened limit ($S \rightarrow 0$), the metal Fermi level becomes pinned to the semiconductor CNL. CNLs, like MIGS, are a fundamental property of a semiconductor, so they do not change with geometry or type of metal. However, one of the simplest silicide junctions, (111)Si:NiSi₂, does not follow this rule; its A and B interfaces have SBHs differing by 0.15 eV [8], with only a small change in the second nearest neighbour geometry. Secondly, the slope of the experimental SBHs of silicides is steeper than that of the parent metals, and is offset upwards (Fig 1).

Tung [9] proposed a second theory of SBHs, in which it depends on the polarity of the interfacial bonding. However, interfacial dipoles cannot explain the SBH shift at Si:NiSi₂ interfaces because the bonding in NiSi₂ is *non-polar* as seen from the valence charge density (Fig. 2a). Hence, what does control SBHs in silicides, and can we obtain greater control of silicide SBHs for high mobility semiconductors?

2. Model

NiSi₂ has the fluorite structure and is lattice matched to Si. At the (111)Si:NiSi₂ interface, the Si sublattice is continuous across the interface. The NiSi₂ lattice terminates at a 7-fold Ni site, while the Si sites remain 4-fold bonded across the interface. The only difference is that the A interface has ABC stacking, whereas the B interface has a stacking fault.

We note that the highest filled state on the silicide side is a 'dangling bond' on the last Ni site, and that this points at a closer Si atom in the B interface (Figs 3a,b). This interface state is the origin of the different dipole at the B interface [10,11]. Thus, the Fermi level of the metal silicide is not 'pinned' at the CNL of Si. Why not?

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:NiSi₂ 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:NiSi₂. 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 YSi₂ are lattice matched to Si. This has a hexagonal lattice with the metal sites forming planes and the silicons 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:YSi₂ 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:Fe₃Si. 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

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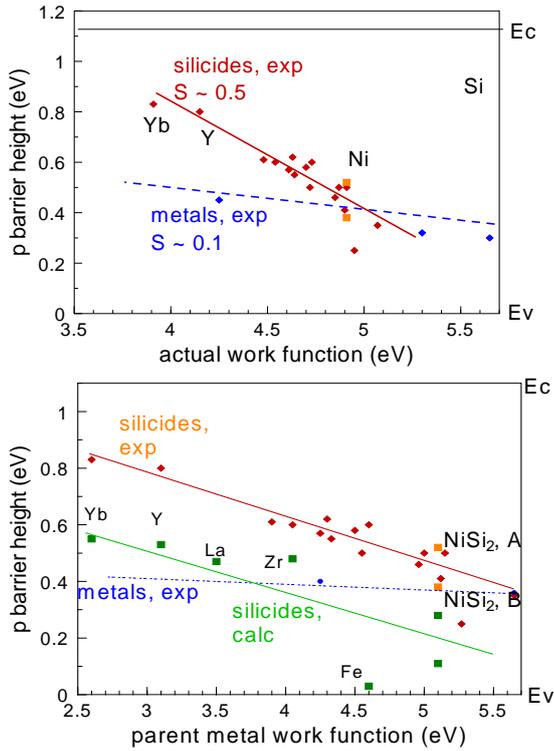


Fig. 1. Experimental Schottky Barrier heights of silicides [4] and pure metals [6] on Si, plotted against (a) actual work function and (b) work function of parent metal, compared to silicide SBHs calculated by LDA. Note that LDA points lie lower in the gap than experimental values due to LDA band gap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

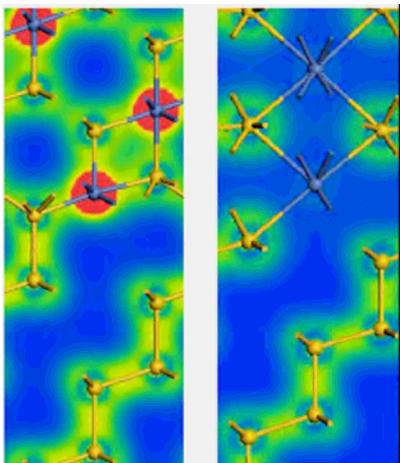


Fig. 2(a) Valence charge density of Si:NiSi₂, with a non-polar spread between Ni and Si sites. Large charge density near Ni is the 3d electrons. (b) Valence charge density of Si:YSi₂ with valence charge localised near Si in the silicide.

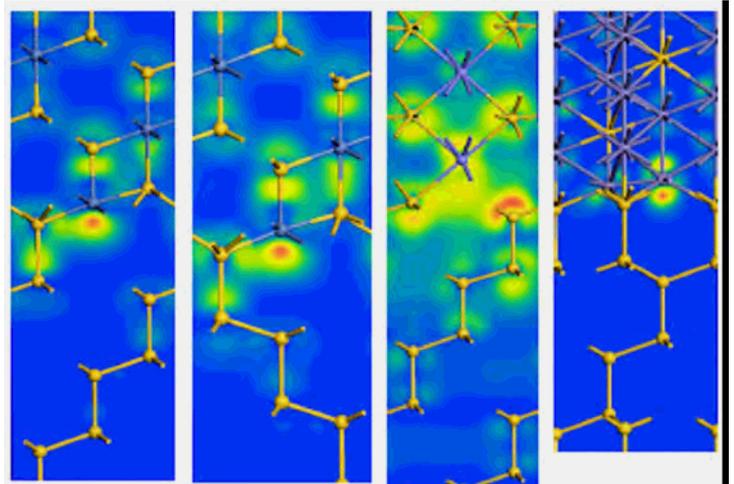


Fig. 3. Highest occupied state for (a) NiSi₂ A, (b) NiSi₂ B, (c) YSi₂, (d) Fe₃Si.

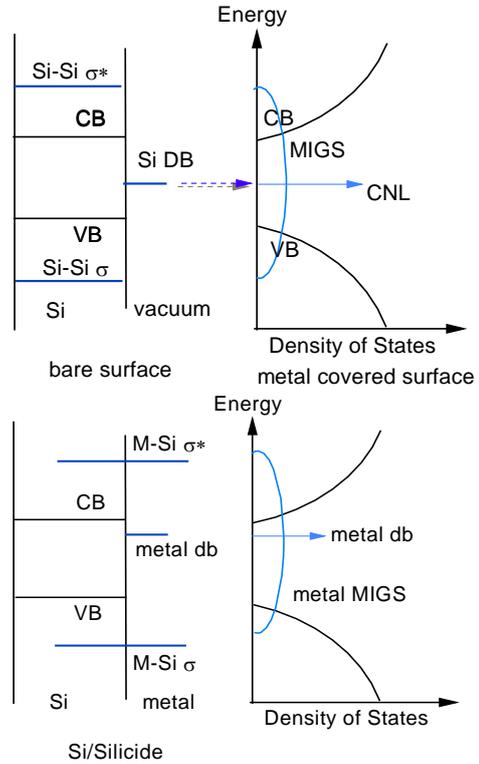


Fig. 4(a). How surface Si dangling bonds develop into MIGS on a metal covered surface. (b) For a silicide interface, all Si DBs are bonded to metal atoms, leaving *metal DBs* to form the interface states. Metal DB energies vary with metal work function, unlike a CNL.