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Mechanism of Ohmic Contacts on Sb- and Bi-based layers on Si and Ge

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1. Abstract

Experimentally, thin films of semi-metallic Bi on Si or Ge enable over-lying metals to form ohmic contacts to the Si or Ge [1]. The underlying mechanism is unclear. We show that it occurs because the inserted Bi layer causes Fermi level depinning of the top contacts. Bi and Sb structures are effectively layer materials, which, in few layer form, have a band gap. Their Fermi level pinning factor is calculated to be S = 0.4 rather than S ~ 0. Hence metals of high or low work function can give low Schottky barrier heights, and depinning.

2. Introduction

Contact resistances of metals to Si and Ge nano-devices limit their performance due to the large Schottky barrier heights, particularly for n-Ge [2]. This occurs because the metal's Fermi level E_F is pinned within a narrow energy range in the gap, so that varying the metal will not lower the barrier height. Various strategies have been tried to overcome this effect, such as inserting thin oxide layers to depin E_F [3,4] or using rare-earth silicides rather than elemental metals [5]. However, while oxide layers do depin E_F, they also insert a series resistance, with little net reduction of contact resistance [4]. Silicides do lower the n-type barrier height but are not so easy to implement for nano-scale devices like FinFETs.

It was recently found that Bi could help to depin E_F [1]. This may be a more easily implementable technology. Here, we explain the underlying mechanism of this effect.

3. Results.

There are two basic models of the Fermi level pinning at Schottky barriers without defect states, Fig. 1. (a) charge transfer from metal-induced gap states (MIGS) to the free electron states of the metal contact [6], (b) or polarisation of the interfacial bonds between the semiconductor and metal, equivalent to charge transfer across these bonds [7]. These two mechanisms lead to a similar dependence of SBH on metal work function, but they are different. In (a) electrons transfer from states at E_F, in (b) they transfer within occupied bonding states. Normally, the density of states at E_F, $N(E_F)$ is proportional to the total valence electron density, N, so the two models are closely related and it may not matter which is chosen.

Sb and Bi have the A7 crystal structure forming puckered atomic layers held together by weaker inter-layer bonds. In bulk, they are semimetals. In few-layer form, they have a gap. We use Sb, to omit spin-orbit coupling.

The band structure of monolayer Sb can be derived from graphene's, Fig 2a, which consists of π states and σ states, and its π states cross at E_F at the K point. Silicene is a monolayer of Si but buckled not a layer as in graphene. From above, it still has the hexagonal lattice, and so its valence and conduction bands cross at E_F at K points, Fig 2(b) [8], like graphene. It is a semi-metal. However, buckling makes the bands not pure π-like, so they are much narrower than in graphene, and lie deeper below the σ states.

Antimonene (β-Sb) has a similar structure to silicene with puckered layers, Fig 3. E_F now lies above the π*-like bands to accommodate its extra valence electron, and the bandgap is between the π* and σ* bands, Fig. 4. Monolayer Sb has a gap of ~1.2 eV in GGA or 2.2 eV in HSE.

If other metals are deposited on top of the few layer Sb (on Si or Ge), these form the external contacts. As the work function [9] of these metals varies, the degree of Fermi level pinning determines how the Schottky barrier height (SBH) varies with respect to the Sb band edges. We calculated these SBHs using the density functional theory, with supercells of slabs of metal atoms on Sb to find the SB pinning factor $S = d\varphi/d\Phi$ where φ is the p-type SBH and Φ is the work function of the contact metal. We find S= 0.4 for monolayer Sb, Fig. 5, compared to S ~ 0.05 for a bare Si surface. That is, a thin Sb layer has depinned E_F, as in experiment [1]. We find that S = 0.2 for metals on few layer Sb (Fig. 6), less than for a monolayer. This is because this Sb has a band gap of only 0.3 eV.

Fig 7 shows the atomic configuration of metal Re, and the quasi-metal MoO_3 on bulk Sb. Here MoO_3 and WO_3 are chosen as high work function degenerate semiconductors (metals) that do not react with the substrate and thus can be confident to form a good interface for DFT calculations.

The S values of 0.41 for a monolayer and 0.2 for bulk Sb show how the S factor of ML Sb is larger than that of Si, but decreases for bulk Sb due to its reduced band gap.

4 Discussion

Sb or Bi have a low density of states at E_F, much lower than in Al, Fig. 8, so it is not proportional to the total valence electron density. In this case, E_F becomes unpinned, and allows E_F to be varied by external metals to give low SBHs. A similar effect occurs for insertions of graphene under metal contacts [10].

Using Sb or Bi as an intermediate contact may be pref-

erable to using oxides, silicides or graphene to lower contact resistance.

References

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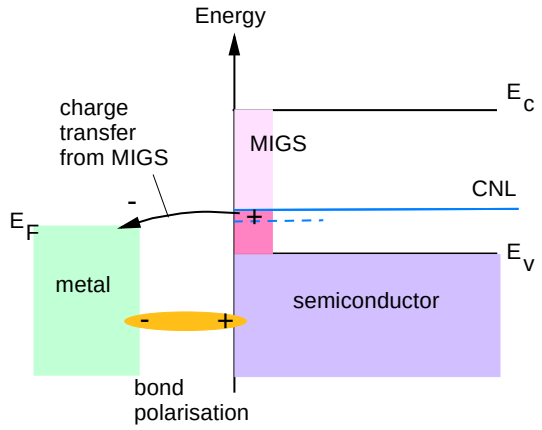

Fig. 1. A metal – semiconductor interface, showing the two different charge transfer mechanisms, (a) from MIGS to metal E_F and (b) polarization of interfacial bonds. In simple free-electron metals, these 2 mechanisms scale with each other. In semi-metals like Sb, Bi they do not., and low density of state at Ef allows Fermi level de-pinning.

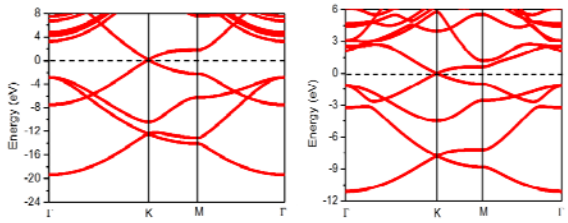

Fig. 2. Band structure of (a)graphene and (b) silicene.

Fig. 3. Side view of the monolayer Sb structure

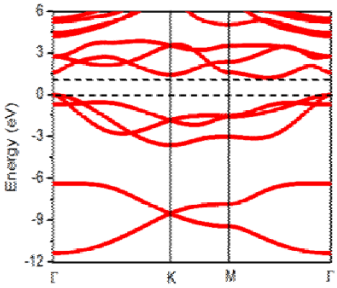

Fig.4. Band structure of monolayer Sb, showing band gap. Band edges shown by dashed lines.

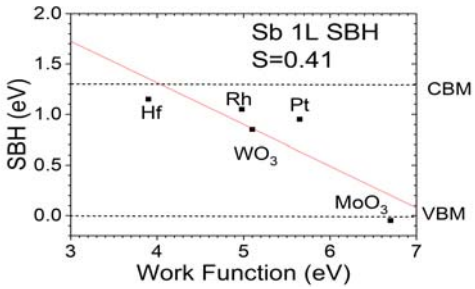

Fig. 5. Calculated Schottky barrier heights on monolayer Sb, with slope S=0.41.

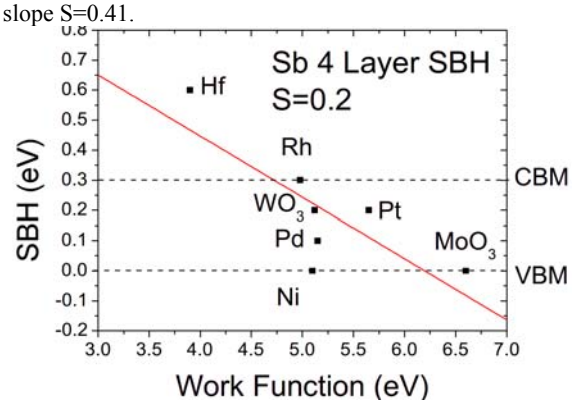

Fig 6. Calculated Schottky barrier height for metals on 4 layer Sb.

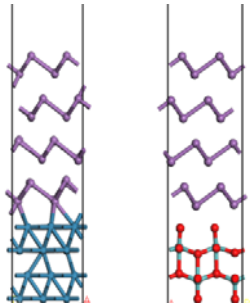

Fig. 7. Relaxed atomic lsyout of Re and MoO_3 layers on Sb.

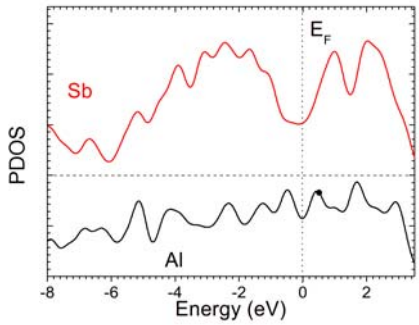

Fig. 8. Comparison of the DOS of the free-electron metal Al, and semi-metal Sb.