Extended Abstracts of the 2020 International Conference on Solid State Devices and Materials, VIRTUAL conference, 2020, pp53-54

Origin of Fermi Level De-Pinning of Metal Silicide, Rare-earth arsenide, TiN and Bi Schottky Barriers

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1. Abstract

The Schottky barrier heights of transition metal silicides on silicon, rare-earth arsenides on GaAs, N-rich TiN on Ge, and Bi on Ge depend more weakly on work function, showing 'Fermi level depinning' (FLD) compared to elemental metals. These metals have an underlying covalent lattice causing mis-coordination defects at interfaces, which create localized interfacial defect states, as well as standard metal-induced gap states (MIGS), and give rise to a sequence of pinning levels which mimic the effect of FLD, but no reduction of total density of states as shown in classic FLD.

2. Introduction

Contact resistances of metals to Si and Ge nano-devices limit their performance due to large Schottky barrier heights (SBHs), particularly for n-Ge [1]. There are three typical strategies to reduce contact resistances, (1) insertion of ultra-thin insulator layers to attenuate the MIGS intensity entering the semiconductor [2], (2) use high doping level to reduce the depletion distance for tunneling, and (3) direct tuning of the SBH by depinning E_F. As there is no nett lowering of resistance by method (1)[3], and (2) is reaching its limits, there is much interest in Fermi level pinning (FLP) and how de-pinning could be used to directly tune SBHs.

3. Results

Metals normally show strong FLP at Schottky barriers due to a high density of states of MIGS [4]. Silicides like $TiSi_2$ to $NiSi_2$ show a much weaker SBH dependence on work function than elemental metals experimentally [5,6] (Fig 1). Rare-earth arsenides like rocksalt-structure ErAs on GaAs show a large variation of SBH for Ga- or As- terminated interfaces [7]. TiN contacts normally act as a constant work function, but if deposited under N-rich conditions, they can show depinning [8]. Finally, Bi shows a depinning and an orientation dependence of its SBHs [9].

All these compound metals have an underlying covalent or ionic lattice, whose interfaces with covalent semiconductors like Si create coordination defects (Fig 2). Bi is a weak metal with low $N(E_F)$ but it also has an underlying covalent lattice leading to lattice mismatch defects with Si.

Our supercell calculations find that interfaces to possess coordination defects. These defects give rise to localized interface states, beyond the MIGS model, Fig 3. Whereas MIGS only decay in the semiconductor, the interfacial defect states decay both towards the metal *and* semiconductor. The states create a higher DOS in the gap, above the MIGS background (Fig 4). This extra DOS causes a 1.2 eV shift of SBH for Ga- and As-terminated YAs/GaAs(100) interfaces (Fig 5-7) [10], impossible in any MIGS model.

For silicides, the extra DOS of interfacial defects (Fig 4) acts to pin E_F at a different energy for each silicide, at an energy that varies more strongly with transition metal than allowed by the MIGS rule. Thus the interface is apparently 'depinned', as E_F shifts strongly with metal species. But it is *not* depinned in the conventional sense, of reducing the MIGS DOS [11]. Also, the new pinning energy can vary strongly with orientation (Fig 1), whereas MIGS pinning energies are independent of orientation in a cubic case [12].

The same behavior could arise for N-rich TiN. TiN's underlying lattice is ionic. TiN is reasonably lattice-matched to Ge. Excess N can create dimer-like N interstitials. These can introduce extra localized gap states that could shift the TiN E_F above its usual mid-gap energy (Fig 8)[8,13]. But TiN has too many reactions, from scavenging to off- stoichiometry to know its response in any specific case.

In Bi (modeled by Sb), mismatch creates an array of defects and localized states. These are not as intense as in a silicide case, but the low $N(E_F)$ of this weak metal strengthens their effect, causing FLD (Fig 9).

4. Conclusions.

Overall, FLD due to localized interface states is found in four systems, and is recognizable due to its orientation dependence, not found for MIGS-based SBHs. However, its depinning is not classical depinning, as there is no lowering of $N(E_F)$. But the right choice of materials system can lead to a pinning energy at the desired band edge, and reduction in contact resistance, the ultimate objective.

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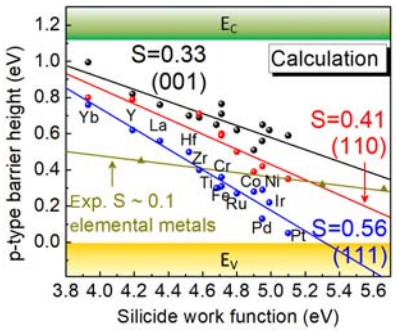

Fig. 1. Calculated SBHs of silicides on (111), (100), (110) Si faces using DFT, with different slopes. Strong pinning of elemental metals, for ref.

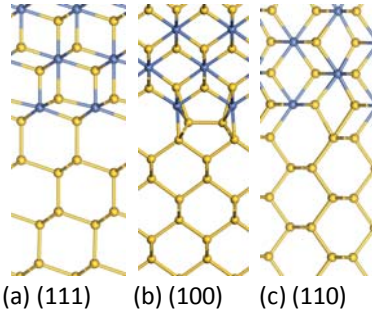

Fig. 2(a) structures of NiSi2/Si(111), (b) NiSi2/Si(100). (c) NiSi2/Si (110) interfaces showing defect sites.

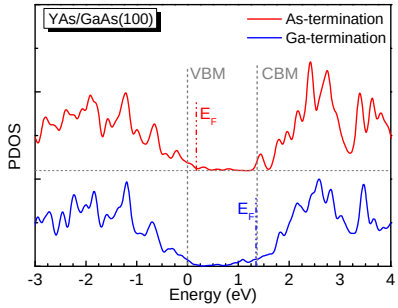

Fig.6. 1.2 eV difference of SBH for Ga- and As-terminated YAs/GaAs(100) interfaces.

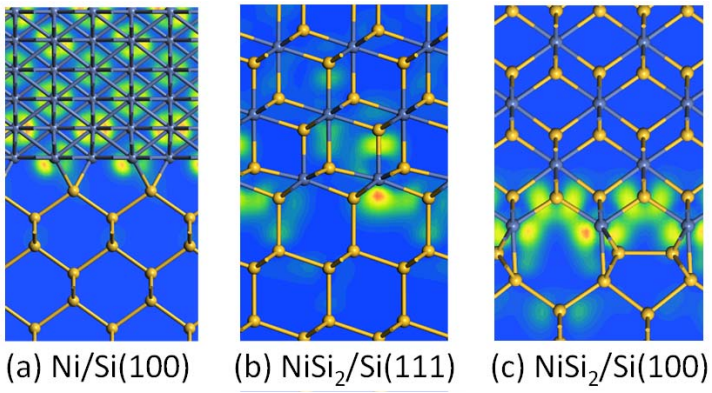

Fig. 3. Wavefunctions near E_F for (a) simple (100)Ni/Si, (b) (111)$NiSi_2$/Si, and (c) 2×1(100)$NiSi_2$/Si interfaces. The silicides show a state localized in both directions from the interface. MIGS in (a) shows no decay on metal side.

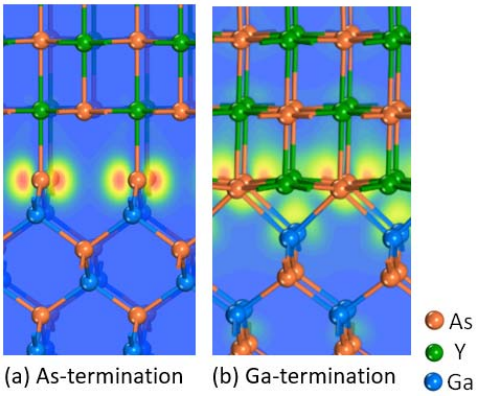

Fig. 7. Localized states at YAs/GaAs(100) interfaces.

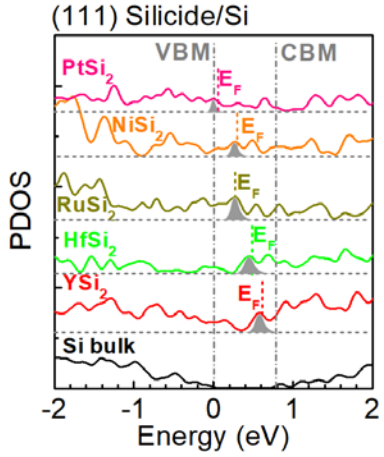

Fig. 4. PDOS of the interfacial layer silicides at (111)silicide/Si supercells. The defect energy is mimicked by a grey shape.

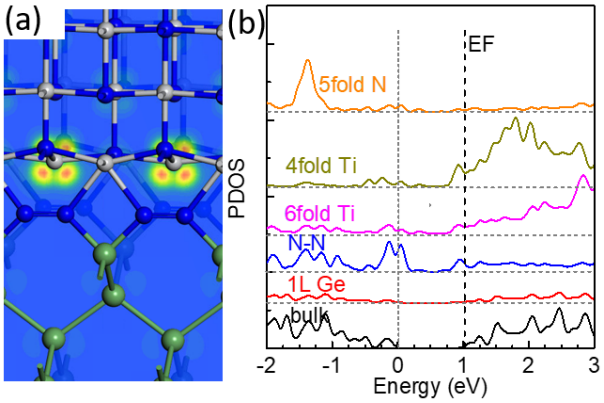

Fig 8. Localized states at 4-fold Ti sites and N-N dimer interstitials, can pin Ef near CBM.(N=blue)

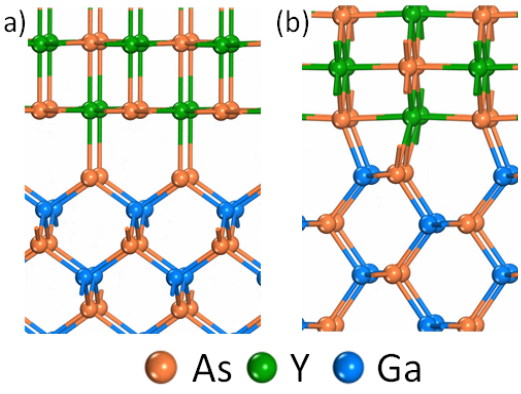

Fig. 5 Structures of Ga- and As-terminated (100)YAs/GaAs. YAs models ErAs to avoid f states.

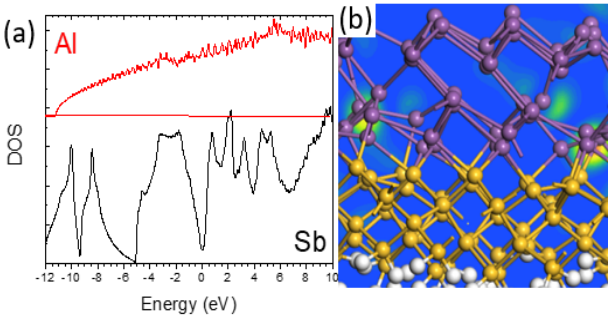

Fig 9. (a) DOS of bulk Sb compared to free-electron Al, (b) Sb on (110)Si showing localized interface states.