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APPLICATION NOTE

Prediction of Schottky Barrier in Electronic Devices

The contact resistance between metals and semiconductors in nanoelectronic devices is mainly determined by the Schottky barrier. Controlling the Schottky barrier height (SBH) hence means being able to manipulate the contact resistance. and thereby to reduce the energy consumption as well as the heat production of electronic devices. While so far phenomenological considerations were able to determine the SBH only at a qualitative level, a parameter-free quantitative evaluation is possible via atomistic simulations using the MedeA® software platform.. This application note illustrates the calculation and modification of the SBH for a system of direct technological importance, namely a NiSi/Si contact. Furthermore, the effect of dopant atoms on the SBH, which are needed to tune the SBH for minimal contact resistance of n- and p-doped semiconductors, is investigated. Reduction of the Schottky barrier height is achieved by doping with Ba. This note also demonstrates how the preferred positions of dopant elements can be determined with S as example.

Keywords: Semiconductor, contact resistance, Schottky barrier, density of states, core level shifts, MedeA®, VASP, hybrid functionals

Formation of Schottky barriers

Schematically the formation of a Schottky barrier is shown in Fig. 1. In metallic materials such as NiSi the highest occupied and the lowest unoccupied electronic state are found at the same energy, namely, the Fermi energy. In contrast, the occupied valence band and the unoccupied conduction band of semiconductors are separated by a band gap as illustrated in Fig. 1. When a metal and a semiconductor are brought into contact, bonds are formed between the two materials, atoms are moving and electrons are redistributed at the interface until equilibrium is reached. As a result the bands of the semiconductor are aligned with the Fermi level of the metal with a particular offset. An electron moving from the metal to the bottom of the conduction band of the semiconductor has to overcome an energy barrier, Φ_{bn}, which is called the Schottky barrier (see Fig. 1). Holes at the top of the valence band of the semiconductor that move to the metallic region need to overcome the barrier Φ_{bp}. For a well behaving effective potential both energy barriers add to the band gap, $\Phi_{bn} + \Phi_{bp} = E_g$.

Atomic arrangement at NiSi/Si interface

For silicon the (100) surface is the technologically most important one. In practice, NiSi is formed by depositing a thin layer (about 30 nm) of Ni onto a Si substrate followed by annealing at 550 °C for about 1 minute[1]. This process involves an interdiffusion between Ni and Si and the formation of NiSi leads to a fairly sharp metal/semiconductor interface.

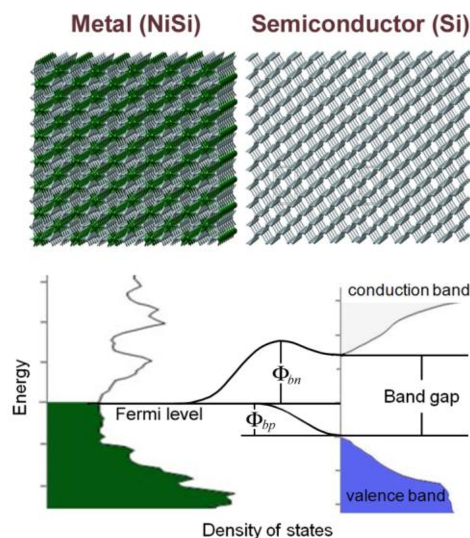

Figure 1. Scheme of a Schottky barrier, Φ_{bn} and Φ_{bp} between a metal and an n- and p-doped semiconductor, respectively.

A model of an (unreconstructed) Si(100) surface is readily created with the MedeA® surface builder tool and then subject to similar treatment as in practice:

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simulated annealing using MedeA® VASP. The resulting structure is shown on the left side of Fig.2.

Electronic Structure of NiSi/Si

The computed alignment of electronic states for the NiSi/Si interface is displayed in the lower part of the left hand side of Fig. 2 in terms of the layer-decomposed density of states (LDOS). Inside the NiSi region the LDOS has the form of that of bulk NiSi and, correspondingly, the LDOS inside the Si region is that of pure Si bulk. The calculations reveal that the Si bands align such that the Fermi level of the metal ends up near the middle of the Si band gap. The effective potential rises smoothly so that the Schottky barrier height Φ_{bn} is the difference between the bottom of the conduction band and the Fermi level. The rise of the potential is monitored by the computed Si-2*p* energy levels shown for each layer of the NiSi/Si interface at the bottom of Fig. 2. The computed value of the SBH, Φ_{bn}, is 0.62 eV, which is in excellent agreement with the experimental value of 0.65 eV reported in Ref. [1].

Electronic Structure of NiSi/Ba/Si

MedeA® predicts the effect of dopant atoms near the interface, as for example Ba, on the SBH.

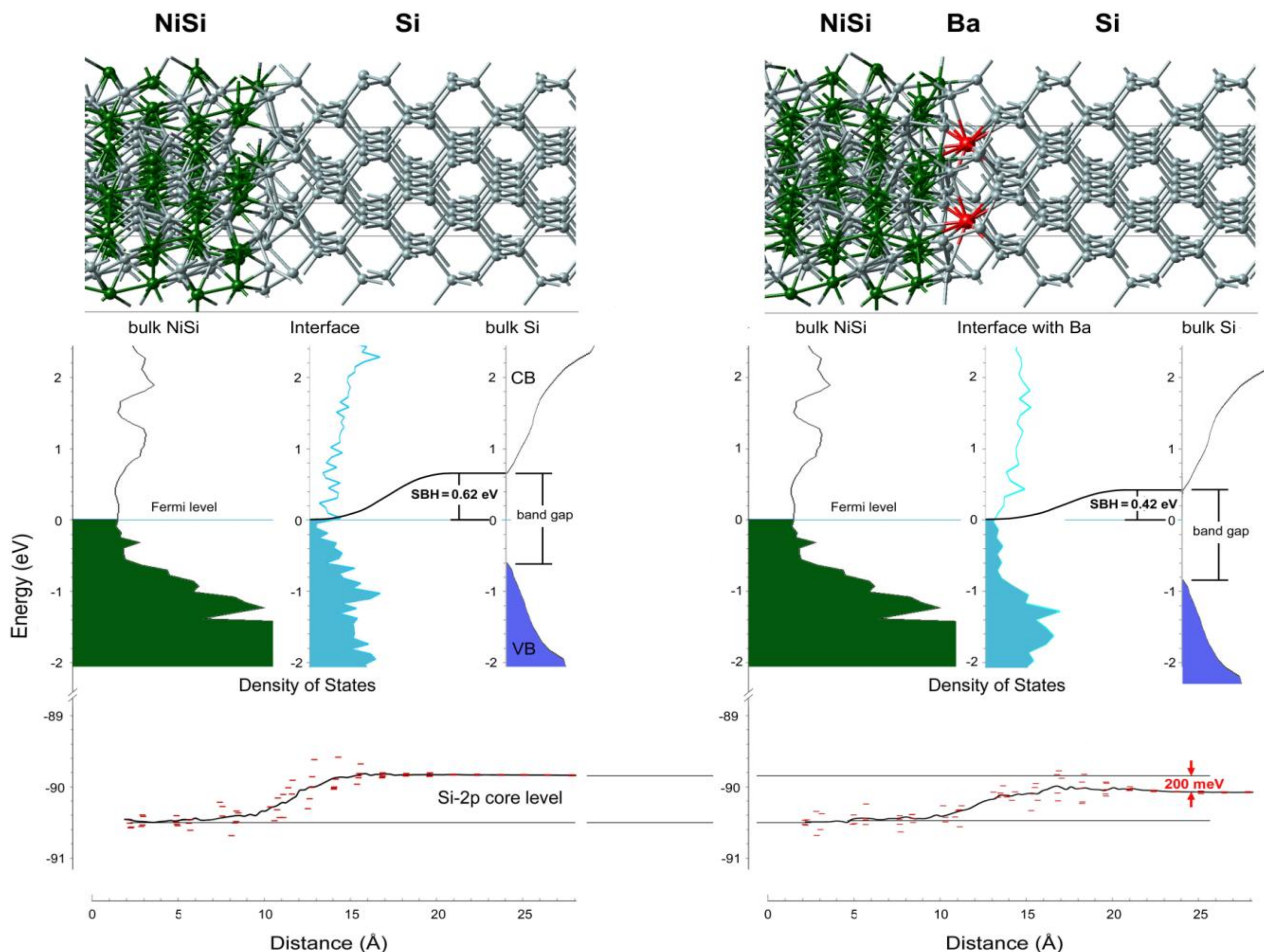

Figure 2. Atomic structures of the interfaces NiSi/Si and NiSi/Ba/Si (top), layer-decomposed density of states -LDOS (middle), layer-decomposed Si-2p energy states (bottom). Inside the NiSi phase and inside the Si layers the LDOS is that of the corresponding bulk material with the computed alignment. The LDOS for Si atoms in the interface region is given in the middle. CB — conduction band, VB — valence band.

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In general the effect of the dopant atoms is most conveniently monitored by shifts in the Si-2*p* energy levels inside the Si region relative to the reference energy levels inside NiSi. As shown in Fig. 2, the calculations reveal that the electronic energy levels inside the Si are shifted by 200 meV to lower energies relative to the reference levels inside NiSi. As a consequence, the valence band minimum moves closer to the Fermi level and the SBH Φ_{bn}, is reduced from 0.62 eV to 0.42 eV.

Location of dopants at the NiSi/Si interface

Using the atomistic simulation techniques of MedeA® the energetically most stable positions of any dopant atom or impurity can be examined. In case of NiSi/Ba/Si it was assumed that the dopant atom is located near the interface, but *a priori* it is unknown where dopant or impurity atoms are located. For instance, calculations on NiSi/Si interfaces with sulfur impurities show that the S atoms energetically prefer the region near the interface, but also could remain inside the silicide. They are energetically less stable inside bulk Si. If S is implanted into Si prior to the formation of nickel silicide, it is likely that during the silicidation process S atoms accumulate at the NiSi/Si interface, but also get incorporated in the NiSi phase. The role of sulfur in tuning the SBH in NiSi/Si systems is an area of active research[2].

Significance

Atomistic simulations with MedeA® have a high predictive power in controlling the contact resistance in electronic devices. Electronic structure calculations, which can be routinely performed using MedeA® VASP, are increasingly employed industrially (see, for example, the patent application from Toshiba[3]). The need for an atomistic level understanding is amplified by the increasing materials diversity and the decreasing dimensions of modern electronic devices.

The methodology[4] implemented in MedeA® is generally applicable in case of a large number of different materials, interfaces, and dopants, thus providing a unique tool for the interpretation of existing experimental data and, perhaps more importantly, for focusing new experiments on the most promising candidates.

MedeA® Modules Employed in this Case

The present calculations were performed with the MedeA® features and modules

- MedeA® environment
- MedeA® Interface Builder
- MedeA® VASP
- MedeA® JobServer and TaskServer

References

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