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A Role of Ultra Thin Silicon Interlayer in Au/Si/*n*-GaAs Contacts: Depinning of the GaAs Surface

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1. Introduction

The III-V compounds based metal-semiconductor (M-S) contacts are essentially independent of the metal work function irrespective the Schottky model. A reason for that is believed to consist in interface states introduced by defects on the interface or owing to the proximity of the metal. Of recent decade, tuning of Schottky barrier height (SBH) in a quite wide interval has been achieved via an ultra-thin, preferably heavily doped Si interlayer inserted between the semiconductor and Schottky metalization [1-7].

The possible mechanism responsible for the SBH tuning is still a matter of discussion and conflicting models are reported. The essential crux in question seems to be weather a role of the silicon interlayer consists in interface state density reduction at the Si/GaAs interface (thus unpins the Fermi level), or a new pinning position is established. Chambers and Loebs [5] reported that epitaxial growth of undoped Si on GaAs does not unpin the Fermi level in the sense of a significant reduction of the interface state density. In contrast, unpinning of the Fermi level from its mid-gap value is proposed by other authors [1,2]. Band-structure calculations performed recently confirmed this influence of silicon overlayer provided its thickness is below ca 15 Å [9].

We present a photoemission spectroscopy study on electrical properties of *n*-GaAs(001) surface modified by deposition of the undoped silicon overlayer with thickness d_{Si} covering quite narrowly the interval from ca 4 to 25 Å. The view was extending to study the SBH versus d_{Si} dependence.

2. Experiment

The starting material was *n*-type GaAs(001) epi-layer with the doping concentration of n=1.5×10^{16} cm^{-3} grown on the substrate in the 10^{18} cm^{-3} doping range covered by a thick amorphous passivating arsenic cap-layer. The cap was thermally desorbed under ultrahigh vacuum (UHV) conditions. Both the decapping and the following Si evaporation were performed at 330°C. Silicon film was deposited from an undoped high purity silicon rod, while the As partial pressure was below the detection limit of about 5×10^{-11} mbar. The structure was topped by evaporation of thin gold layer with the thickness of ca 16 Å further thickened to about 100 Å.

3. Results and discussions

An inspection of valence band spectra revealed a double leading edge incidental to the valence band offsets of GaAs and Si overlayer; Fig.1 manifests spectra for two different overlayer thickness' (middle and bottom spectrum) along with the spectrum of the bare GaAs surface measured before the silicon deposition (upper). We observed no influence of the silicon overlayer thickness on the valence-band disconti-

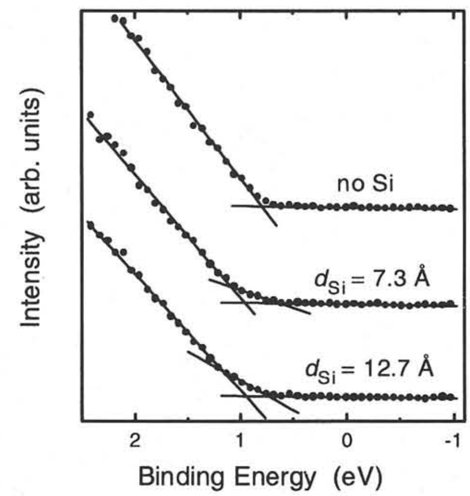

Fig.1 Valence-band photoelectron spectra for a clean GaAs surface (top) and for the GaAs surface covered by 7.3 Å -(middle) and 12.7 Å -thick (bottom) silicon overlayer. The solid lines are least squares fits to the data.

nuity within the inspected range; the offset appeared to be constant of 0.29 ± 0.05 eV, relatively close to experimental value of 0.39 ± 0.1 eV already reported by Bratina *et al* [3]. Restricted to the value only, one can not incline in favour of any of the most agitated models, since they are in serious conflict in their assumptions, but the predicted band discontinuities appear to be similar for the Si/GaAs interface. More specifically, the electron-affinity rule model [10] predicts 0.27, model by von Ross [11] gives 0.30 eV, and the quantum dipole-based model [12] concludes 0.34 eV.

The change of the GaAs surface Fermi level after Si deposition was inferred from both the Ga *3d*-core level shifts and from the E_F-E_{VB} distance as well. The band bending, as deduced from the Ga *3d* core-level shift (see Fig.2, left axis), decreases by about 0.24 eV in comparison to the value observed for the decapped surface, if the silicon thickness of ca 10 Å has been achieved. Beyond this thickness, Fermi level returns towards to the middle of the gap. This tendency of Fermi level shift was confirmed by the valence-band

*On leave from Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, SK-842 28 Bratislava, Slovakia inspection (not shown here) and is at variance with observation reported in Ref.[5], where band bending remained unchanged after the undoped silicon layer growth. We suppose, the flattening of the band-bending is due to interface state density reduction [13].

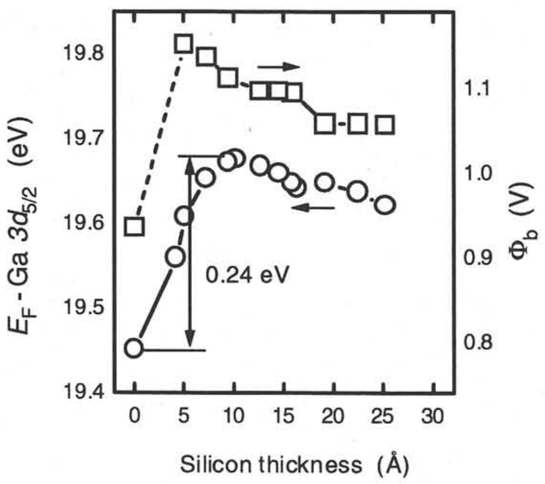

Fig.2 The evolution of the Ga *3d* core-level shifts (left axis) after silicon deposition and SBH of the Au/Si/*n*-GaAs(001) structures (right axis) versus the silicon interlayer thickness. The connecting lines are only a guide for the eye.

Fig.2 also compiles the SHB development with the silicon interlayer thickness (right axis), as calculated via the relation $\phi_B = E_g - (E_F - E_{VB}) - \Delta E_{BB}$, where ΔE_{BB} is the change in the band bending. The SBH peaks for $0 < d_{Si} \leq 5$ Å, but no data are available within this interval to specify a maximal attainable SBH and its corresponding silicon thickness. Beyond 5 Å, monotonous decrease of the SBH occurs. We already observed such non-monotonous dependence of the SBH on interlayer thickness recently [8].

If we direct our attention to the thickness interval $5 < d_{Si} \leq 10$ Å, a decrease in both the interface state density and the SBH occur at the same time. The theoretical value for SBH follows from the Schottky-Mott relationship $\phi_B = \phi_M - \chi$, given for an ideal metal/*n*-type semiconductor contact. The Au work function ϕ_M found in the literature ranges from 5.1 to 5.45 eV [14, 15] in dependence of the preparation conditions and measurement methods. Taking into account these values, the Schottky limit of Au/*n*-GaAs contact (supposing electron affinity χ of GaAs being of 4.07 eV) should be within the range from 1.03 to 1.38 V. The decrease of the SBH to the value of ca 1.1 V according to our observation can be interpreted as SBH's *approach* to the value predicted by the theory for interface states-free contact. The model in the framework of the interface state reduction induced by interlayer has been previously applied to Si-based structures [16].

We stress that even undoped silicon overlayer results in marked change of the band-bending. About 2 ML's were reported to be enough to saturate final stage [6]. Hence, structural models of Si/GaAs structure reposed upon bulk silicon properties [2] seem implausible, since interface properties must play a major role, as also pointed out in e.g. Refs. 6 and 9. We suppose, the heavily doping (dopant incorporation is comparable to silicon growth rate [6] and mixed alloys are even formed [7]) preferably used to tune SBH influences the silicon layer properties, but even more dramatic changes of GaAs surface must be induced through surface stoichiometry departure at the same time (introduced purposely e.g. in Ref.4). Likely, various models can interplay depending on the interface preparation.

4. Conclusions

In summary, we measured band-bending of GaAs(001) surface modified by the undoped Si overlayer growth and the SBH evolution induced by the interlayer as well. Employing a combination of Fermi level and SBH versus silicon thickness dependencies we conclude that the SBH tendency for silicon thickness less than 10 Å can be explained as an approach to the Schottky limit predicted for the ideal metal-semiconductor contacts due to decrease of interface state density at the Si/GaAs interface.

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