

Electronic structure of silicon based heterojunctions used for solar cells

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Heterostructures have inherent advantages over homojunctions. Generally it is possible to combine the advantageous properties of materials involved in heterostructures, to realise a controlled modification of the heterojunction interface and to make a bridge between organic and inorganic solids.

The application of heterostructures leads to a cost reduction of pn-junction cells (thin film, EFG silicon, low thermal budget) and establishes new working principles like hot carrier injection structures.

What are the key problems which we have to solve for keeping all the expectations?

- (1) Atomic-chemical state of the interface (diffusion, intermixing, reaction, topography),
- (2) Modification of the growth and basic properties of ultrathin layers (substrate interaction, initial stage of growth, quantum effects),
- (3) band (molecular orbital) adjustment and their modification by buffer layers
- (4) interface state distribution, band bending, recombination,
- and (5) charge transfer processes and scattering of hot electrons.

By means of selected results from our research we will illustrate the relevance of the key problems and some of their consequences for application. This shows that a preparation and analysis on an atomic depth scale is required. On the other hand, we need barrier energy sensitive methods like internal photoemission (IPE) and/or ballistic electron emission microscopy (BEEM). We investigated these methods and found a correspondence in the measured internal yields which can be explained by the fact that both methods are dominated by scattering and interface reflection processes of the hot electrons. This has remarkable consequences for the application of these methods and the interpretation of their results.

Our research activities are focussed on silicon based hetero solar cells like TCO/a-Si/c-Si and TCO/c-Si solar cells. One interesting point is the interaction of oxygen with silicon during the growth of TCO layers on silicon. This was investigated by applying an atomic radical source as an oxygen supplier with variable ion/atom ratio and ion energies. XPS measurements give an insight into the silicon oxide growth by detection of the chemical shift of the Si2p line. It results that the silicon oxide formation at low temperatures is an strongly ion assisted process. The formation of silicon suboxide species can be avoided at elevated temperatures. The barrier energy of the formed contact between TCO and silicon was analysed by IPE. Degeneration of In₂O₃ at the contact region with silicon was not always observed. The defect structure and the atomic chemical state of the initial stage of TCO growth is still under investigation.

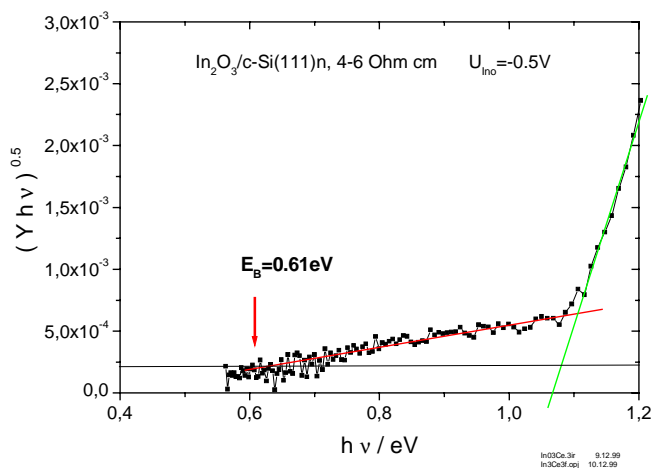


Fig. 1 Modified Fowler plot of the photoinjection quantum yield vs. the photon excitation energy.

$E_B=0.61$ eV marks the barrier energy for electrons between the degenerated thin In₂O₃ (30nm) and c-Si(n).

The energetic distribution of gap states, interface states and the band offsets play a crucial role for the heterostructures. The detection of these quantities is possible by photon excited electron emission if the escape depth corresponds to the top layer thickness. The excitation with photon energies below 10 eV results in an increase of the escape depth up to 10nm. Strong monochromatic UV-light (3-7eV) was used for the Constant Final State Yield Spectroscopy measurements of the gap state distribution of phosphorous doped and undoped a-Si:H emitter layers deposited on c-Si. The increase of $N(E)$ with the doping and the shift of the Fermi level towards the conduction band is shown in Fig.2.

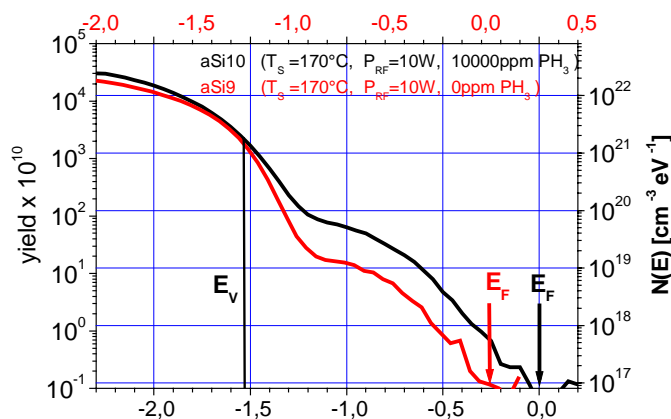


Fig2. Density of states $N(E)$ vs. the bonding energy E_B detected by UPS from a n-doped and an undoped a-Si:H layer. The a-Si:H layer thickness amounts to 10nm. The red curve is shifted by -0.3 eV.

We will discuss the obtained changes of $N(E)$ as a function of doping, their consequences for the Fermi level position and the Urbach energy in such thin amorphous layers. For comparison we use the classical method of photoconductivity yield at thick (120nm) a-Si:H layers to detect $N(E)$ in a direct manner. The a-Si:H gap states interact with the adjacent c-Si by tunneling and directly influence the recombination at these interfaces. This was shown by photoluminescence measurements at differently prepared a-Si/c-Si heterojunctions.

A future perspective for low temperature emitter layers are organic materials. We found that the organic material/c-Si(111) and organic material/c-Si(100) heterointerfaces are well passivated. We deposited benzene compounds and PPV electrochemically or by spin coating on the Si surfaces. The lowest interface state densities obtained from surface photovoltage measurements are below $1 \cdot 10^{11}$ states $\text{eV}^{-1} \text{cm}^{-2}$ at midgap.

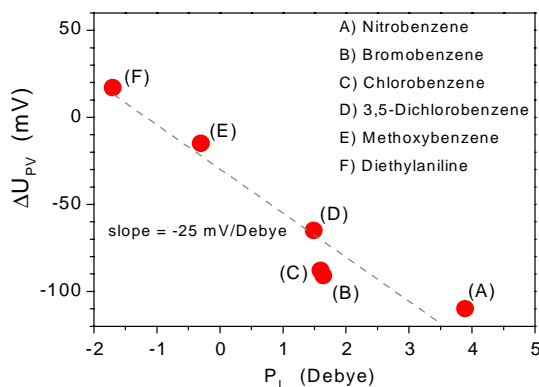


Fig.3 Band bending of Si surface, $q \cdot \Delta U_{PV}$ as a function of the electrical dipole momentum for different benzene compounds, P_{\perp} , perpendicular to the surface as measured during electrochemical deposition.

The band bending of the silicon surface can be adjusted by the dipole moment (compound dependent) of the first organic monolayer (Fig.3). Attempts to use this concept for efficient heterojunction solar cells failed because the charge transfer through the organic layer, their HOMO/LUMO band adjustment and the coating by TCO are critical and patchy solved up to now. Under the aspect of heterojunction requirements we apply our analytical and preparative methods to get more insight in these central questions of a organic/inorganic heterojunction.