# Chapter 8

# Schematic Density of States

In Chapter 4-7, a study of electronic states located in the band gap of $\mu$c-Si:H using different experimental techniques and conceptional methods was described. However, all these experiments have certain limitations and therefore provide information only in a limited range. The aim of this section is to combine this information into a schematic picture of the density of states in both a spatial and energetic sense.

From the results obtained in the study of hole drift-mobilities in highly crystalline $\mu$c-Si:H it could be deduced that the disorder within the investigated material is sufficient enough to strongly alter the band-edge states and affects the charge carrier transport. Applying the model of multiple trapping it could be shown that the band-tail falls exponentially towards the gap with a band width of $\Delta E_V \approx 31$ meV. The existence of conduction band-tail states could be observed by the well known CE resonance found in n-doped $\mu$c-Si:H material, but neither the shape nor a typical width can be derived from these data. However, recent investigations using photoluminescence suggest that an exponential distribution also applies for the conduction band-tail [75].

The ESR signal of intrinsic microcrystalline silicon shows an asymmetric line shape which can be described by two Gaussian distributions db$_1$ and db$_2$ at g-values of g=2.0043 and g=2.0052, respectively. The results presented in this work suggest that these contributions are independent states located in different microscopic environments. So far the exact location of the states remains unknown. However, combining the results obtained in this work some speculations can be made. The energetic position within the band gap can be determined from the study of n-type material presented in Chapter 5. Together with the data derived from transient photocurrent measurements presented in Chapter 7, a schematic picture of the density of states for highly crystalline material can be drawn, as shown in Fig. 8.1 (a). To provide a comprehensive view on the DOS, the energetic distribution of the db$_1$ and db$_2$ states within the band gap has been included,
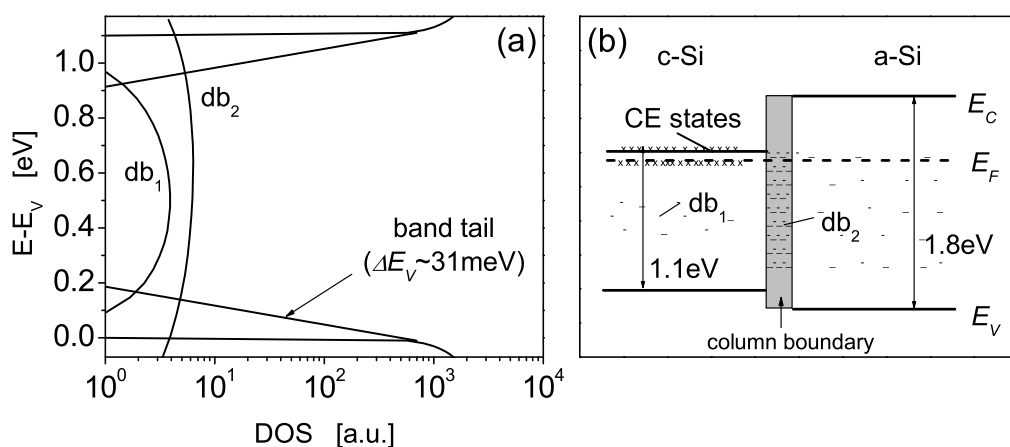
**Figure 8.1:** *(a) Schematic picture of the DOS of highly crystalline material as derived from the results of this work. The distribution of the $db_1$ and $db_2$ states below mid-gap has been taken from reference [30] and [40]. (b) Schematic band diagram of the transition region between the crystalline and disordered phase in $\mu c$-Si:H (see the text for details).*

that have been taken from reference [30] and [40], respectively. It can be seen that the energy distribution of the $db_1$ signal is rather concentrated within the crystalline gap of $E_G = 1.1$ eV, while the $db_2$ resonance strongly overlaps with the conduction band-tail. It was therefore suggested, that the $db_2$ resonance in highly crystalline material are spatially separated from CE states presumably located at the columnar boundaries. This was also concluded in earlier investigations [165]. Additional support for this thesis comes from the study of intrinsic $\mu c$-Si:H prepared at different $T_S$. Due to the higher deposition temperatures hydrogen desorbs during the process. As there are a number of indications that the bonded hydrogen is located at the column boundaries, terminating dangling bond defects, it is therefore tempting to relate the higher $N_S$ to a poor surface passivation caused by the hydrogen desorption. In Chapter 4 it was argued that the increasing $N_S$ is borne by an increasing number of $db_2$ states, suggesting that these states are located at the column boundaries. The assignment of the $db_2$ resonance to surface states located at the column boundaries is supported by the reversible effects on the ESR signal investigated in Chapter 6. These processes were attributed to the adsorption of oxygen at the columnar clusters. As the adsorption mainly effects the occupation of near surface states, the change of the $db_2$ resonance indicates that the origin of this line are states within this region. Quite surprisingly, the $db_1$ resonance at g=2.0043 stays unaffected by these processes. On might therefore conclude that the origin of these states is within the crystalline columns, which is in agreement with an energetic distribution confined within the crystalline band gap. In conclusion, one can draw a schematic band diagram for microcrystalline

silicon as shown in Fig. 8.1 b, which illustrates the transition between crystalline and amorphous phase in $\mu$c-Si:H. It is important to note, that the amount of both phases varies considerably as a function of the deposition conditions. While in material exhibiting the highest crystallinity no amorphous phase can be observed and the structure consists only of crystalline columns and column boundaries, well beyond the transition to amorphous growth crystallites are highly diluted in an amorphous matrix.

All results summarized in this section indicate that majority of $db_2$ states are located at the columnar surfaces, while the states resulting in the $db_1$ resonance are located within the crystalline grains. With increasing hydrogen or amorphous content the spin density decreases, indicating that $db_2$ states can be passivated by hydrogen, with an amorphous tissue around the crystallites acting as a passivation layer.