Chapter 9

Summary

In the present work, the electronic properties of microcrystalline silicon films have been studied by using various experimental techniques and a number of concepts and models used to explain them. Paramagnetic states in μc-Si:H have been investigated for a large variety of structure compositions ranging from highly crystalline, with no discernable amorphous content, to predominantly amorphous material, with no crystalline phase contributions. For this material range, the density of states within the band gap was studied by electron spin resonance (ESR) and electrical conductivity. Moreover, the hole transport properties in highly crystalline material were studied by transient photocurrent measurements and have been successfully interpreted by the model of multiple trapping in an exponential band-tail.

The spin density N_S in μc-Si:H films is strongly dependent on the structure composition of the material. The highest N_S is always found for material with the highest crystalline volume fraction. With increasing SC during the process, the spin density decreases, which was attributed to an increasing hydrogen content, terminating unsaturated dangling bonds. Moreover, the additional amorphous phase content incorporated between the crystalline columns acts as a passivation layer, leading to a better termination of unsatisfied bonds at the surface. The strong dependence of N_S on the deposition temperature T_S, found in HWCVD material, was attributed to an increasing desorption during the deposition.

Generally, the ESR signal of intrinsic microcrystalline material shows contributions of two resonances at g-values of 2.0043 (db_1) and 2.0052 (db_2), independent of the particular deposition process and structure composition. The relative contributions of the individual lines changes as a function of the crystalline volume content. While the ESR spectra of low defect material in the highly crystalline regime are dominated by the resonance at g=2.0043, with increasing amorphous content the intensity ratio is clearly shifted towards the db_2 resonance. An

increasing intensity of the db_2 resonance is also observed as a result of increasing T_S.

Reversible and irreversible changes in the ESR signal and the conductivity found in μc-Si:H due to atmospheric effects are closely connected to the structure composition, in particular the active surface area. The porous structure of highly crystalline material leads to the in-diffusion of atmospheric gases, strongly affecting the density of surface states. Two processes have been identified, namely adsorption and oxidation. Both processes lead to an increase of N_S. In the case of adsorption the increase could be identified as arising from changes of the db_2 resonance, while the intensity of the db_1 resonance remains constant. With increasing amorphous content the magnitude of both adsorption and oxidation induced changes decreases as a result of a higher compactness of the films. The adsorption of O_2 may be reversed by moderate temperature annealing, while a chemical treatment in HF is required to reverse the effects caused by oxidation.

Measurements on n-doped μc-Si:H films were used as a probe for the density of gap states. The results confirm that the doping induced Fermi level shift in μc-Si:H, for a wide range of structural compositions, is governed by compensation of defect states for doping concentrations up to the dangling bond spin density. For higher doping concentrations a doping efficiency close to unity is found. It could be shown that in μc-Si:H the measured spin densities represent the majority of gap states ($N_S = N_{DB}$). The close relationship between the CE resonance intensity and the conductivity is confirmed, which means the electrons contributing to the CE signal represent the majority of the charge carriers contributing to electrical transport.

Transient photocurrent measurements were carried out on μc-Si:H material prepared in the highly crystalline regime. It was found that in these materials conventional time-of-flight interpretation is consistent and may be applied to obtain hole drift mobilities. It has been shown that in this material hole transport is dominated by effects associated with multiple trapping in valence band-tail states. Analyzing the transient photocurrents it was found that the density of valence band-tail states falls exponentially towards the gap with a typical band-tail width of $\Delta E_V \approx 31$ meV.

Combining the information derived in this work a schematic picture of the density of states in both a spatial and energetic sense has been obtained.