Abstract

Layers of $Fe_{1-x}Co_xS_2$ with $x \leq 0.1$ are grown by metal-organic chemical vapour deposition (MOCV) on substrates of glass, silicon and natural pyrite and characterised. T-butyl disulfide, iron pentacarbonyl and tricarbonyl nitrosyl cobalt are used as precursors. With the exception of some layers, grown on natural single crystalline pyrite substrates, the layers are polycrystalline with grain sizes ranging from 50 to 500 nm. The chemical and structural composition is analysed by X-ray- and ion beam methods. Cobalt is incorporated in the lattice on iron sites proportional to the fraction in the gas phase during the deposition. Except for the pyrite structure with a slightly increased lattice constant no other crystal phase is detected.

For sufficiently high cobalt concentrations ($x \geq 3 \cdot 10^{-3}$) the layers exhibit n-type conductivity. The transition from p-type conductivity of undoped layers to n-type conductivity of cobalt doped layers is indicated by the turn over of the Seebeck-coefficient as well as by the occurrence of a negative Hall-coefficient. For high carrier concentrations $n = 6 \cdot 10^{20}$ cm^{-3} Hall measurements allow the determination of carrier densities. For all cobalt concentrations the samples exhibit a semiconducting behaviour and the bandgap decreases with increasing cobalt concentration by about 100 meV for x = 0.1.

At room temperature cobalt doped samples show Hall mobilities in the range of $\mu_e = 0.1 ... 5$ cm^2/Vs. The temperature dependence of the carrier mobility can be explained by a model, where the charge carriers are thermally emitted over the grain boundary barriers. They are induced by acceptor type traps at the grain boundaries. The trap density, here estimated for the first time for polycrystalline n-type doped pyrite, is about $N_t = 10^{13}$ cm^{-2} in the examinated doping range. This is about one order of magnitude higher than reported for other semiconductors, e. g. polycrystalline silicon. With lower doping concentrations smaller trap densities might occur depending on the energy position of the trap states in the bandgap. However, according to the XPS-results this is not to be expected.

The photoactivity of the doped layers is proved by a significant increase of the signal amplitude of microwave reflection at excitations with laser light of 1047 nm and 523 nm.

Subsequent thermal treatment at 600 °C under sulphur atmosphere results for doped as well as for undoped layers in an increased grain size and decreased carrier concentration and conductivity.

The epitaxial deposition of n-type doped pyrite layers on natural monocrystalline substrates was successful, but – due to lack of suitable p-type substrates - only on n-type substrates. p-n junction of (001)-textured $Fe_{0.99}Co_{0.01}S_2$ layers on p-type substrates show identifiable but weak diode behaviour.