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Origin of unusual Ag diffusion profiles in CdTe

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Radiotracer experiments are the most sensitive tool for the study of diffusion phenomena in solids. At ISOLDE/CERN diffusion experiments have been performed using 111-Ag delivered for implantation by ISOLDE. It has been shown that in CdTe 111-Ag exhibits the phenomenon of uphill diffusion, which under suitable conditions (800 K, 60 min, Cd-pressure) results in the formation of symmetric concentration-depth profiles that are strongly peaked about the center of a several 100 μ m thick crystal [1,2]. The phenomenon of uphill diffusion is quantitatively understood and successfully described by a theoretical model [3,4] leading to the conclusion that the dopant profile essentially images the profile of the deviation of stoichiometry generated by the diffusion of Cd-interstitials into the initially Te-rich CdTe crystal.

Uphill diffusion can be observed also at significantly lower diffusion temperatures down to 450 K, if metal layers are evaporated onto the implanted surface of an initially Te-rich CdTe crystal [5]. We assume that a Cd-rich layer between the metal and the CdTe crystal is formed, which is responsible for the in-diffusion of Cd-interstitials into the Te-rich material. This creates a deviation of stoichiometry, which is imaged by the dopant, leading to the uphill profiles.

In addition, it is possible to image a profile of the deviation of stoichiometry generated before the implantation of the radiotracer. For this purpose a metal layer was evaporated onto the surface of a CdTe crystal, which subsequently was annealed at a temperature of 470 K. After removing the metal layer by etching, 111-Ag was implanted followed by annealing at 550 K in order to diffuse the dopant. The 111-Ag dopant showed an uphill diffusion profile as expected.

The experimental data indicates that the composition of the surface present during the annealing process influences the diffusion of the 111-Ag dopants significantly. This is further supported by experiments showing that uphill diffusion can be initialized also by an etching procedure leaving behind a Cd-rich surface. In contrast, this seems not to be the case if an etching procedure creates a Te-rich surface.

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Primary author: LEHNERT, Johannes (Experimentalphysik, Universität des Saarlandes, 66123 Saarbrücken, Germany)

Co-authors: WOLF, Herbert (Experimentalphysik, Universität des Saarlandes, 66123 Saarbrücken, Germany); JOHN-STON, Karl (Experimentalphysik, Universität des Saarlandes, 66123 Saarbrücken, Germany); DEICHER, Manfred (Experimentalphysik, Universität des Saarlandes, 66123 Saarbrücken, Germany); WICHERT, Thomas (Experimentalphysik, Universität des Saarlandes, 66123 Saarbrücken, Germany)

Presenter: LEHNERT, Johannes (Experimentalphysik, Universität des Saarlandes, 66123 Saarbrücken, Germany)

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