Optical properties of isoelectronic centers in crystalline silicon

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Citation for published version (APA):
Summary

This thesis deals with fundamental properties of selected optically active isoelectronic centers in silicon.

The radiative decay of excitons bound to isoelectronic impurities is an important physical process in crystalline semiconductors. This is particularly true in indirect band-gap semiconductor like GaP, Si, in which the band-to-band radiative transitions are forbidden by the $k$-conservation rule. Therefore motivation for the presented study comes from practical importance of silicon photonics as the way for integration of electronic and optical elements. In addition, exciton bound to copper or silver related centers in Si. and Er dopant which can receive energy by binding an exciton can emit infrared light at a wavelength of around 1.3 $\mu$m or 1.5 $\mu$m, which is most suitable for transmission by glass-fiber. In the first Chapter of this thesis, some general aspects of the isoelectronic centers are discussed and the experimental techniques used in this work are summarized in Chapter 2.

The results of a detailed phenomenological study of the optical properties of a silver-related center in silicon have been reported in Chapter 3. Perturbations of optical transitions by uniaxial stress and magnetic field have been accurately described in terms of an effective-mass electron, orbiting the center in a triply degenerate orbital state of $T_d$ symmetry, and a tightly bound hole, which has its angular momentum quenched by the local trigonal field of the center. Using effective mass for vibrational mode derived from isotope data, the electron-phonon coupling of a reasonable magnitude is obtained. With this model, the total luminescence and the radiative decay time have been fitted over the 4 - 50 K temperature range. It has also been shown that the data can give an estimate of the time necessary to thermally ionize an electron from an effective-mass state. A detailed phenomenological understanding of the optical properties is therefore achieved, even though the molecular structure of the core of the center has not been determined.

Chapter 4 illustrates how the ionization cross section can be measured for centers of unknown concentrations from time-resolved two-color excitation measurements. The value obtained for a copper center in silicon is verified by comparison with the absorption coefficient reported for shallow donors of a well-defined concentration. Further, the presented data demonstrate a partial recovery of the luminescence after photo-ionization, due to repopulation of the ionized traps.

The first observation of Zeeman effect in PL of Si:Er system has been reported in Chapter 5. This provides the most direct microscopic information on the structure of a prominent center responsible for optical activity of Er in crystalline silicon. From a clear magnetic field induced splitting observed on the main line of the Er-1 PL spectrum, the lower than cubic symmetry of the emitting center is
conclusively identified as orthorhombic-I ($C_{2v}$), with $g$ tensor of the ground state of $g \equiv 18.39 \pm 0.81$. $g_\perp \equiv 0$. On the basis of these findings, the paramagnetism of the Er$^{3+}$-related center emitting at $\lambda \approx 1.5 \mu m$ is unambiguously established, and the understanding of the important and notoriously difficult Si:Er system is significantly advanced.

Chapter 6 presents results of a complete magneto-optical study of multinanolayer Si/Si:Er structures grown by SMBE technique. The presence of Si spacer regions considerably increases emission intensity when compared to that of single layers. The PL of annealed multinanolayer structures is dominated by emission from a particular center, the Er-1 center, which is then preferentially formed. The PL spectrum of this center is characterized by ultra narrow homogeneous lines. Based on analysis of the magnetic field induced, angular dependent splitting of the PL lines, we confirm the orthorhombic-I symmetry of the Er-1 center and give $g$-tensors for several lower-lying levels of the $^4I_{15/2}$ ground and the lowest excited $^4I_{13/2}$ state multiplets. In particular, we identify the original $\Gamma_6$ and $\Gamma_7$ characters for the lowest crystal-field split levels of the ground and the excited states, respectively. Based on the study, the microscopic structure of the Er-1 center is proposed. It comprises a single Er$^{3+}$ ion at a distorted interstitial $T_d$ site with multiple oxygen atoms in its direct vicinity.

A detailed consideration of excitation mechanisms of the Er-1 center in multinanolayer Si/Si:Er structures prepared by SMBE under cw and pulse laser pumping is carried out in Chapter 7. The overall excitation cross section for Er$^{3+}$ ions is determined as $\sigma = (6 \pm 2) \times 10^{-15} \text{ cm}^2$. This high value implies that excitation of the Er-1 center is a very efficient process. Further, by a direct comparison with a calibrated SiO$_2$:Er sample, it has been concluded that up to $\sim 32\%$ of the total number of Er$^{3+}$ ions present in Si/Si:Er nanolayers can attain optical activity. This represents a considerable improvement over Si:Er prepared by ion implantation and, as discussed in the introduction paragraph of this Chapter, opens new hopes towards realization of optical gain in Si:Er.

The influence of a $p$-$n$ junction created by Er implantation at a Si/Si:Er interface on the PL excitation kinetics of the Er$^{3+}$ ions has been analyzed in Appendix A. It is shown that dissociation of excitons by the electric field potential at the junction can explain the delayed onset of Er PL, when excited from the non-implanted side of the silicon wafer. This finding confirms that excitons are responsible for excitation of Er$^{3+}$ ions in crystalline silicon at low temperatures.