

Defect annealing in TiO₂ (rutile)

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TiO₂ has a wide range of applications. It is used as pigments in paints, sunscreen and food products, and as a photocatalyst, where doping by ion-implantation has been found useful to tailor the photocatalytic properties. TiO₂ is used as a host for the upconversion process and in recent years there have been reports on dilute magnetism in this system, where the charge state of Fe is of importance.

A study of the annealing processes and charge state of dilute Fe in rutile TiO₂ single-crystals was performed in the temperature range 143-662 K, utilizing on-line ⁵⁷Fe emission Mössbauer spectroscopy following low concentrations (<10⁻³ at.%) implantation of ⁵⁷Mn ($T_{1/2} = 1.5$ min.). Both Fe³⁺ and Fe²⁺ were detected in the entire temperature range. Three annealing stages were distinguished:

- i) A broad annealing stage below room temperature leading to an increased Fe³⁺ fraction.
- ii) A sharp annealing stage at ~330 K characterized by conversion of Fe³⁺ to Fe²⁺ and changes in the hyperfine parameters of Fe²⁺, attributed to the annealing of Ti vacancies in the vicinity of the probe atoms.
- iii) An annealing stage in the temperature range 550 to 600 K, where all Fe ions are transformed to Fe³⁺, attributed to the annealing of the nearby O vacancies.

The dissociation energy of MnTi-VO pairs was estimated and Fe³⁺ found in a paramagnetic state with slow spin-lattice relaxation which does not follow the expected T² dependence expected for a Raman process.

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