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HELVETICA PHYSICA ACTA

Zusammenfassungen der letzten eingegangenen Arbeiten
Résumés des derniers articles reçus

Effect of Crystal Orientation on a $\gamma\gamma$ Angular Correlation in ^{166}Er

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(16. VIII. 71)

Solid State Reactions and Defects in Doped Verneuil Sapphire

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(27. VIII. 71)

Abstract. Extending earlier work on Ni and Co doped sapphire to Ti, Fe and doubly doped (Fe, Ti) sapphire the phenomenon of non additive color of multiply doped corundum was given special attention. Since in all these cases Verneuil grown crystals show dopant inhomogeneous distribution, local concentrations were determined by electron microprobe analysis calibrated by neutron activation analysis. Polarized and high resolution UV-VIS spectra, polarized IR and quantitative ESR spectra of the doped crystals in the untreated state and after oxidation by O_2 and reduction by H_2 at 1500°C are given. Information derived therefrom shows Ti to be present as Ti^{+3} and Ti^{+4} , Fe as Fe^{+2} and Fe^{+3} and (Fe, Ti) as $(\text{Fe}, \text{Ti})^{+6}$ and $(\text{Fe}, \text{Ti})^{+7}$ in the reduced state and oxidized state respectively. In the reduced state hydrogen is shown by polarized infrared spectra and isotopic shifts to occupy an interstitial site between two O^{-2} ions of the larger oxygen triangles on (001) planes. For assignment of the UV-VIS bands near 385 and 450 nm of $\alpha\text{-Al}_2\text{O}_3$: Fe^{+3} extended crystal field calculations were carried out based on a point charge lattice, using all $3\text{ }d^n$ electron configurations of Ti^{+3} and Fe^{+3} and Hartree-Fock atomic orbitals for free ions. In order to obtain acceptable agreement between observed and calculated spectra the quantity $\langle r^4 \rangle$ is considered as a fitting parameter, leading to considerably higher $\langle r^4 \rangle$ values for both Ti^{+3} and Fe^{+3} . Under this assumption an assignment for the $\alpha\text{-Al}_2\text{O}_3$: Fe^{+3} spectrum compatible with the observed polarization and high resolution UV-VIS data may be given. The characteristic and nonadditive spectrum of $\alpha\text{-Al}_2\text{O}_3$: (Fe, Ti) in the reduced state is shown by various arguments to originate from a biparticle $(\text{Fe}, \text{Ti})^{+6}$. Finally thermodynamic data for redox reactions and relatively detailed models for the substituted ions in different oxidation states are given.