ORDER-DISORDER STRUCTURAL TRANSFORMATIONS IN NANOCRISTALLINE HIGHLY IMPERFECT R2TIO5 (R = Er, Tm, Yb, Lu) FLUORITE DERIVATIVES

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Recently it was found that single-crystalline and polycrystalline samples of R_2MO_5 (R = Gd, Y, Sc; M=Ti, Zr, Hf) contain nanodomains (10–600 nm in dimension) with different degree of order, coherent with the fluorite-like matrix[1-2]. In this research order-disorder phenomena in $xR_2O_3 \cdot (1\text{-}x)TiO_2$ (R = Er, Tm, Yb, Lu; 0.5≤x≤0.6) solid solutions with highly imperfect fluorite-derived structures have been studied using monochromatic synchrotron X-ray diffraction and Raman spectroscopy. The results demonstrate that the synthesis process leads to the formation of two coherent cubic phases identical composition: disordered fluorite-like (*F*) phase (*Fm3m*) and with different degrees of ordered pyrochlore-like (*P*) phase (*Fd3m)*, which consist of nanoscale (<100 Å) and nanocrystalline domains. The cubic fluorite-derived phases *F* (*Fm3m*) and *P* (*Fd3m*) have similar lattice parameters in a fluorite setting. It is, therefore, reasonable to believe that the crystal lattices of fluorite and nanocrystalline domains of the pyrochlore phases are coherently joined through transition layers created by dislocations, staking faults, microtwins, and other structural defects. In the compositions range of the solid solutions (0.5≤x≤0.6), the lattice parameter of the fluorite-like phase follows Vegard's law. The formation of nanodomains with different degrees of order is shown to be caused by the internal strain due to the high density of structural defects in their unit cells.

References
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