Poster Presentation

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Incommensurate modulated structures and luminescence in scheelites

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Scheelite (CaWO4) related compounds (A',A'')n[(B',B'')O4]m with B', B''=W and/or Mo are promising new materials for red phosphors in pc-WLEDs (phosphor-converted white-light-emitting-diode) and solid-state lasers. Scheelites can be prepared with a large concentration of vacancies in the A sublattice, giving compositions characterized by a (A'+A''):(B'O4+B''O4) ratio different from 1:1. The creation of cation vacancies in the scheelite-type framework and the ordering of A cations and vacancies are a new factor in controlling the scheelite-type structure and properties. Very often the substitution of Ca2+ by M+ and R3+ (R3+ = rare earth elements) in the scheelite-type structure leads to switching the structure from 3D to (3+n)D (n = 1,2) regime. The creation and ordering of A-cation vacancies and the effect of cation substitutions in the scheelite-type framework are investigated as a factor controlling the scheelite-type structure and luminescent properties of CaGd2(1-x)Eu2x(MoO4)4(1-y)(WO4)4y (0≤x≤1, 0≤y≤1) solid solutions. Within this series all complex molybdenum oxides have (3+2)D incommensurately modulated structures with superspace group I41/a(α,β,0)00(-β,α,0)00, while the structures of all tungstates are (3+1)D incommensurately modulated with superspace group I2/b(αβ0)00. In both cases the modulation arises due to cation-vacancy ordering at the A site. The replacement of the smaller Gd3+ by the larger Eu3+ at the A-sublattice does not affect the nature of the incommensurate modulation, but an increasing replacement of Mo6+ by W6+ switches the modulation from (3+2)D to (3+1)D regime. Acknowledgement. This research was supported by FWO (project G039211N, Flanders Research Foundation) and Russian Foundation for Basic Research (Grants 11-03-01164, and 12-03-00124).

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