PHASE EQUILIBRIA IN THE BAF_2-YF_3 SYSTEM

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The spectroscopic properties of rare-earth doped BaY_2F_8 (BAYF) have been extensively studied for solid-state laser applications and have been recently investigated for the potential use of this material as a scintillator in radiation detectors; for the latter application, some of BAYF crystals's best properties include a high output light yield and the possibility of tuning the emission to the light detector device by choosing the dopant [1, 2]. In this work, an investigation of the BaF_2-YF_3 binary system was performed with the objective of clarifying the thermal behavior and phase equilibria surrounding the BaY_2F_8 compound, an important requisite for obtaining high quality crystals required for both applications. Several mixed samples of compositions ranging between 58 and 80 mol% YF_3 were synthesized under a reactive atmosphere. The starting compounds were obtained through hydrofluorination of high purity yttrium oxide and barium carbonate. Differential thermal analysis, differential scanning calorimetry, thermogravimetry, X-ray diffraction, scanning electron microscopy and energy-dispersive X-ray spectroscopy were employed in order to characterize the samples. An assessment of the optimal experimental conditions for thermal analysis was required prior to the investigation of the system itself due to the intense vulnerability of YF_3 to oxygen contamination and the problem of the overlapping of thermal events near the melting of BaY_2F_8 [3]. Crystal growth through the zone melting method was also performed in order to examine the system's phase diagram. Results from the many characterization techniques presented important discrepancies with the phase diagrams found in the literature: differences in the phase transition temperatures were observed and evidence that BaY_2F_8 melts incongruently was found. A partial phase diagram that covers the composition range studied in this work and which reflects the observed discrepancies was proposed based on these results.

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