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Growth of Trigonal Gadolinium Fluoride in a Glass-Ceramic for Scintillation and Optical Applications

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Abstract

This work determines the X-ray powder diffraction peak positions for trigonal GdF₃ experimentally and using simulation. An oxyfluoride matrix glass-ceramic containing the inorganic compound GdF₃ was synthesised by quench casting followed by controlled heat treatment. X-ray diffraction analysis was used to confirm the amorphous nature of the as-cast glass, and to identify the compounds crystallised in the glass-ceramic by heat treatment. A simulated powder diffraction pattern for trigonal GdF₃ was calculated and used to confirm the identity of the compound crystallised in the glass-ceramic as being trigonal GdF₃. Rietveld refinement of the structural model was performed using the measured diffraction pattern to accurately determine the unit cell parameters and asymmetric atomic coordinates. A simulated powder diffraction pattern was then calculated for trigonal GdF₃ using the refined structural parameters.

Keywords: gadolinium fluoride, glass-ceramic, scintillator, crystallisation, polymorphism

1. Introduction

Glass-ceramics incorporating scintillating compounds in the form of nano-sized crystallites are being investigated as an alternative to monocrystalline scintillators for gamma-ray spectroscopy applications [1]. Compounds investigated for such scintillators include rare earth fluoride compounds, such as LaF₃, CeF₃,
5 GdF₃, and LuF₃, often doped with rare earth ions. Here, the trigonal polymorph of GdF₃ is investigated.

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