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Numerical time-dependent 3D simulation of flow pattern and heat distribution in an ammonothermal system with various baffle shapes

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Abstract

A numerical analysis of an ammonothermal synthesis process for the bulk growth of nitride crystals was performed. The analysis includes the development of a thermal model for a lab-scale ammonothermal autoclave, which was validated by in-situ temperature measurements and applied to tailor the temperature field inside the autoclave. Based on the results of the global thermal 2D simulations, a local 3D model was used to include convective phenomena in the analysis. Moreover, the influence of the baffle and different baffle shapes on the flow velocity was investigated. Fluctuations of the temperature as well as the flow velocities occur, indicating that 3D considerations are essential to accurately investigate the heat and mass transport in ammonothermal systems.

Keywords: A1: 3D CFD, A2: Ammonothermal, B1: Nitrides

1. Introduction

The ammonothermal synthesis is a promising technology for the growth of high quality bulk nitride crystals e.g. GaN. The growth technique is derived from the hydrothermal synthesis industrially used to grow high quality oxide crystals like α-quartz and ZnO [1]. Instead of water in the hydrothermal technique, the ammonothermal autoclave operates with supercritical ammonia under high pressure and temperature. Inside the autoclave a baffle divides the reaction chamber into two zones the dissolving zone where the raw material is solved in NH_3 and the growth zone where the seed crystals are located. The dissolution of

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