# HYDRODYNAMIC INSTABILITY AND SPIRAL GROWTH OF BULK SINGLE CRYSTALS

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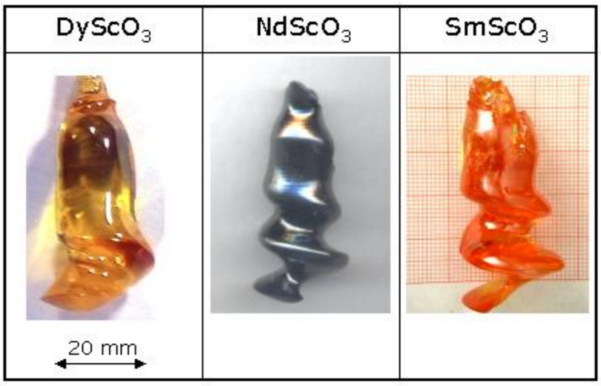
The growth of rare-earth scandates from the melt has become very important during the last few years. These crystals are excellent candidates for substrates of ferroelectric materials (e.g. non-volatile FRAMs). Unfortunately most scandates tend to produce an undesirable spiral structure during the growing process. Even in axisymmetric conditions with axisymmetric initial conditions, a spiral structure can arise via spontaneous symmetry breaking. The figure shows three examples grown at melting temperatures of about 2000°C using the Czochralski method. These high temperatures make internal measurements very difficult and a numerical simulation is required to understand what is happening..

The theoretical approach starts from a 2D axisymmetric solution and considers the stability of the solution with respect to 3D disturbances. This approach gives rise to a set of eigenvalue problems and is similar to that already published by an Israeli group [1]. The eigenvalue calculations can be used to estimate the approximate critical value of a parameter (such as crystal rotation rate) at which the symmetry breaking bifurcation occurs. The bifurcation points can be located exactly using an appropriate extended system of equations, and an effective numerical branch following technique used to compute paths of these bifurcation points as a second parameter is varied. This curve bounds the region in which no instability to spiral growth patterns occurs.




Numerical results in 2D and growth experiments already show the relative importance of several internal and external conditions that influence the flow pattern in the melt in a way to promote or avoid spiral growth. In our assumptions about the basic mechanism of spiral growth (corkscrew instability) the hydrodynamic interaction plays a significant role. It turns out that an analysis of the growth stability can be performed in terms of fluid flow behavior, i.e. a bifurcation study for the hydrodynamic parameters applied to the Navier-Stokes equations. Since the momentum equations are strongly coupled to the thermal conditions including radiation the problem becomes complex and therefore only the most significant parameters have been taken into account. This may happen directly by modifying the flow conditions (rotation rate, crucible shape) or via influencing the thermal environment (thermal absorption in the crystal, shape and location of a baffle). It can be shown that these modifications cause considerable changes of stable and unstable regions in a bifurcation diagram. The regions mark the border lines to be used for real crystal growth processes in order to avoid unstable growth conditions. However, this stability analysis only yields a solution for the limiting case determining the transition to a real 3D solution. The enormous computational requirements for solving sequences of eigenvalue calculations, 2D transient as well as the direct 3D computations can be met by applying a partly iterative solver combined with the fastest currently available direct solver MUMPS [2]. Moreover, recently IKZ became a privileged user of HLRN [3] allowing us to benefit from a total performance of about 5 TeraFlops

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