Numerical study of thermal stresses and dislocation dynamics during growth of oxide and fluoride crystals from melt

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The growth of oxide crystals from melt using the Czochralski, optical floating zone and similar techniques is characterized by high melting points of 2000 °C and higher, causing high thermal gradients in the crystal. The resulting thermal stresses are a well-known problem that leads to degraded structural properties or even crystal cracking during growth or cool-down, e.g. [1]. While thermal stresses and their relaxation by plastic deformation have been investigated for classical semiconductors (Si, Ge, GaAs) using the Alexander-Haasen (AH) dislocation density model [2], similar investigations for oxide and fluoride crystals are rather scarce. In a few studies, the AH model has been applied to chlorides and iodides [3] as well as oxides, such as sapphire [4]. Although the validation of AH model parameters based on experimental data is often lacking, these studies have provided valuable input for further process development.

In the present work, we consider a crystal growth setup for the Czochralski growth of model materials with low-melting points (e.g., $NaNO_3$ or CsI). These experiments were designed to resemble typical growth processes of oxides and fluorides but allow for in-situ measurements, particularly of the temperature field. Measurement data was applied to thoroughly validate 2D and 3D global thermal models [5] and obtain an accurate temperature field in the crystal. The unsteady temperature distribution is imported into the recently developed MACPLAS code [6], which calculates stress and dislocation dynamics in the crystal using the AH model (see [7] for a recent application to Si growth).

In the first step, elastic thermal stresses for different stages of the growth process are calculated for both 2D and 3D cases, considering anisotropic elasticity in the latter case. The accuracy of axisymmetric and isotropic approximations (frequently used in the literature) is evaluated. In the next step, a parametric study based on the 2D, isotropic AH model is performed, considering variations of the most relevant AH model parameters, e.g., the activation energy and coefficients in the dislocation velocity law. The sensitivity of results such as the maximum residual stress in the crystal to the model parameters is examined. In this way, general features of the stress and dislocation fields can be separated from features that show strong model-dependence. While the former facilitates further process optimization, the latter helps to set goals for material characterization.

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