Smart growth, from combined crystal growth methods to artificial intelligence management: control of the chemical composition and improvement of single crystal performance

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Abstract

Nowadays, standard and versatile techniques for growing single crystals from a high temperature liquid phase and using, for instance, the Czochralski, Bridgman or flux processes, are commonly available in worldwide laboratories and dedicated companies for obtaining a wide range of inorganic bulk crystals: oxides, halogenides and semi-conductors. Two categories of materials are usually considered: congruent-melting compounds, which are grown from a melt, and non-congruent-melting compounds, which are grown from a high temperature solution. However, due to intrinsic peculiarities of each technique: thermal distribution, heating medium, possible range of growth kinetics, as well as specific thermomechanical and chemical features of gaseous, liquid and solid phases, as-grown boules with the required quality can display a limited useful volume. Indeed, boules can exhibit local defects such as colour centres, dislocations, chemical vacancies, cracks, impurities or cluster inclusions, which decrease drastically the crystal performance.

On one hand, in order to improve the crystal size and quality with a low rate of defects, we present the combination of different conventional growth methods as a way to achieve the growth of targeted compounds and solid solutions with enhanced compositions, properties and quality. On the other hand, we present a study that integrates machine learning with numerical modeling. The objective is to unravel the nonlinear relationship between crystal growth process parameters and furnace geometry on one side, and solid/liquid interface shape and v/G (growth rate over temperature gradients) on the other side. We exemplify this approach by focusing on defect-free YAG and Ge crystals. Various examples of applications in the fields of optics, piezoelectricity, multiferroics and alkali-ion battery are presented.

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