Marie Sklodowska-Curie fellowship

Point defects in ionic and iono-covalent bulk single crystals

Point defects are of importance in advanced functional materials and especially single crystals. In the case of covalent crystals such as Si or Ge, they are limited to vacancies, interstitials and dopants. Anyhow they control most of the properties of the semiconductor material. It exists an appreciable amount of theory and numerical simulation tools aiming to predict the homogeneity and distribution of point defects in such crystals. The situation is more complicated in the case of binary semiconductors such as GaAs, InP, CdTe and so on. This is due to their binary nature and to the partially ionic character of the atomic bonds: Schottky, Frenkel and other defects appear. Recent developments, based on thermodynamic arguments and calculations, allowed to better understand the behaviour of point defects in such materials.

In the case of **ionic dielectric crystals**, point defects, also known as "colour centres" are at the origin of many useful bulk single crystal applications, such as lasers, optic amplifiers, scintillators, detectors and so on. It is therefore very important to be able to understand, then predict and control, the valence state and distribution of the dopants in the bulk crystal.

Our **research team** is studying the effect of crystal growth parameters (thermal field, melt convection, growth rate …) on the bulk crystal quality (chemical homogeneity, structural defects, residual stresses, grains and twins…). The obtained knowledge allowed optimisation of practically all crystal growth processes, for various crystals: Bridgman (growth of CaF_2 and of BGO), Czochralski (growth of InP and of GaAs), zone melting (SiC from solution in Si), Verneuil (growth of Al_2O_3), shaping (also Al_2O_3). More recently, solidification of photovoltaic silicon. In almost all cases, this has been performed in close collaboration with industry.

The **research project** is aiming to develop a physico-chemical general model of point defects incorporation in ionic dielectric bulk crystals during their growth, possibly with the help of molecular dynamic simulation. This necessitates computation of the local activity of all constituents in the melt and in the crystal all along the growth process, which depends on the local temperature and concentrations. The capabilities of the model will be tested by comparison with measurements performed in industrially grown crystals, such as on figures 1 and 2. A longer fellowship could result in the tentative development of a numerical simulation software able to predict point defect distribution in single crystals after their growth.

Candidates should have strong basis in materials science and thermodynamics. Interest in numerical simulation is welcome but not mandatory.

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SIMAP laboratory, CNRS and Grenoble Institute of Technology will closely assist the applicant in the preparation of the proposal.

Fig. 1: 100m diameter sapphire single crystal doped with Ti for ultra-high power lasers. Courtesy RSA company.

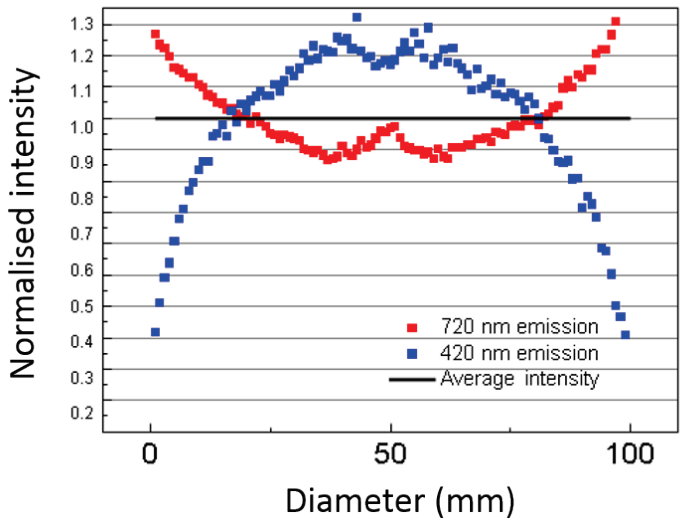

Fig. 2: radial distribution of Ti^{3+} (blue) and Ti^{4+} (red) ions in the crystal.