2019-2020

Master thesis proposal

Institut de Chimie Moléculaire et des Matériaux d'Orsay
Synthèse, Propriétés et Modélisation des Matériaux – SP2M

Title: Single crystal growth of entropy stabilized oxides

Keywords: single crystals, entropy, magnetic properties

Scientific description:
High-entropy oxides (HEOx) or *Entropy Stabilized Oxides* constitute a new class of materials that has been discovered recently by extending to oxides the concept of high-entropy materials that was known since 2000s in the case of metallic alloys. They comprise at least five different cations and are obtained by heating at a high temperature followed by quenching. When the temperature is large enough, the entropy of configuration becomes dominant in the total Gibbs energy $\Delta rG = \Delta rH - T\Delta rS$. Thus, instead of forming phases being driven by the enthalpy of formation, the system crystallizes in a metastable solid solution at high temperature that can be frozen at room temperature by quenching, leading to *entropy-stabilized* materials. HEOx are not only "new materials", but they represent a new paradigm in the design of new functional materials, driven by entropy of configuration.
For the case of (MgCoNiCuZn)O, the first canonical composition reported in 2015 by Rost et al., when a mixture of the binary constituents is heated at temperatures > 875 °C then quenched to room temperature, a simple rocksalt structure where the cations are distributed randomly on the face-centred-cubic sublattice is formed. The formation of such novel structures is governed by entropy thus *enforces* the cations to occupy randomly cationic sites, for instance all five cations listed before occupy octahedral sites. This entails exotic properties, for instance : colossal dielectric properties, ionic conductivities or antiferromagnetic ordering. All these properties were evidenced by our group in Orsay. For this stage we would like to focus on the magnetic properties of these materials. As single crystals are crucial in studying these properties we propose to explore an original method for growing centimeter-size of entropy stabilized compounds, for the first time.

Techniques/methods in use: Solid state chemistry, X-ray diffraction, crystal growth
Applicant skills:
Industrial partnership: N

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Internship location:
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Possibility for a Doctoral thesis: Yes (subject to admission to 2MIB Doctoral School).