NÉEL INSTITUTE Grenoble

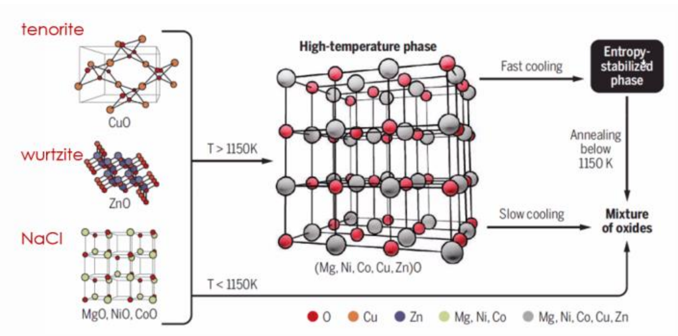
Topic for Master M2 internship – Academic year 2024-2025

New compositions of host crystals for rare earth phosphors: using high-entropy materials to reduce the pressure on rare earth supply chains

General Scope. Owing to their unique luminescent properties and excellent photostability, rare-earth (RE) doped oxide materials have developed rapidly with applications that span from lighting, display, optical amplification to emerging fields such as quantum technologies, biosensing or nanomedicine. One key issue that has emerged in the context of an accelerated energy transition is the cost and availability of rare earth elements in the coming years for usage as emitter (Yb^{3+}, Ce^{3+}, Nd^{3+}) or as host crystal formers for these dopants. We are currently exploring new host crystal compositions in order to decrease the quantity of RE host formers by substitution by non-critical elements or to reduce the pressure on supply chains using lower grade REs from circular economy. During this internship, we will develop high-entropy oxides derived from the $Y_3Al_5O_{12}$ garnet (YAG), well known as lasing medium or used in lighting as color converter coupled to blue LED devices. The project will combine (1) syntheses and thermodynamic studies to establish temperature-composition phase diagrams, (2) multi-scale characterizations and (3) photoluminescence studies to evaluate the performances of these new materials as host crystals.

Research topic and facilities available. Since their discovery (Rost *et al.*, Nature 2015, figure below), high entropy oxides (HEO) have become a promising playground to develop new functional materials. HEOs are generally produced by mixing several binary oxides, five or more, in near equimolar amounts. When heated at a temperature above which the configurational entropy dominates the Gibbs free energy term, a solid solution can be formed even from immiscible oxides.

Here, this concept will be adapted to YAG by considering substitutions in the A site of the $A_3B_2B'_3O_{12}$ garnet structure and by monitoring the crystallization temperature of the mixed oxide using temperature-variable powder x-ray diffraction. The gain in mixing entropy will be quantified from the dependence of the formation temperature with the total number of mixed components.



The influence of the chemical disorder on photoluminescence (PL) properties will be addressed by comparing well-crystallized samples incorporating either 1, 2, 3, 4 or 5 cations on the A site of the YAG structure and doped with a lanthanide emitter. This disorder will be characterized using a wide range of multiscale techniques, from EDS coupled to SEM/TEM imaging for chemical mapping, X-ray diffraction or Raman spectroscopy, in addition to the PL studies. The intern will be trained to carry out all these measurements and to interpret the data obtained with the help of experts. Part of the samples will be synthesized prior to the internship.

Possible collaboration/networking. D. Testemale (MRS research team, NEEL), C. Lepoittevin (MRS, NEEL), A. Ibanez (OPTIMA, NEEL), C. Felix (POM, NEEL), J. Fick (NOF, NEEL)

Possible extension as a PhD. not granted in advance, but we are open to support applications

Required skills. strong interest in material science and advanced spectroscopy techniques, motivation for in situ studies and/or experiments at large facilities (ESRF, SOLEIL synchrotron facilities)

Starting date. Flexible.

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