European Mineralogical Conference
Vol. 1, EMC2012-458, 2012
European Mineralogical Conference 2012

A Nd^{3+} luminescence spectroscopic study on the structural disorder of monazite–(Ce)

C. Lenz (1), K. Ruschel (1), A. Kronz (2), D. Talla (3,1), R. Škoda (3), and L. Nasdala (1)

(1) Universität Wien, Insititut für Mineralogie & Kristallographie, Wien, Austria (christoph.lenz@univie.ac.at), (2) Geowissenschaftliches Zentrum, Universität Göttingen, Germany, (3) Institute of Geological Sciences, Masaryk University of Brno, Czech Republic

We present first results of a study addressing whether Nd^{3+} luminescence spectroscopy can be used to estimate the degree of structural disorder in natural and synthetic monazite–(Ce). Our results show that the degree of disorder, as observed from luminescence band broadening/shifting, generally depends on (1) chemical composition (i.e., structural disorder due to incorporation of non-formula elements) and (2) structural state (i.e., radiation damage, crystallinity, strain/stress). Chemical effects were studied on synthetic orthophospates grown using a flux method, and various natural monazite–(Ce) samples. The latter came from a set of well-characterised samples studied recently by *Ruschel et al. (2012)*. In situ electron microprobe -analyses were done using a JEOL JXA-8900 RL (Universität Göttingen, Germany) and a Cameca SX 100 system (Masaryk University of Brno, Czech Republic) [for details see *Ruschel et al., 2012*]. Room-temperature luminescence measurements were done by means of a confocal Horiba Jobin Yvon LabRam–HR with 632, 532, and 473nm laser excitation.

Recently, *Ruschel et al. (2012)* have investigated the structural disorder of monazite–(Ce) using the broadening of the main Raman band of this mineral (i.e., symmetric stretching vibration of PO_4 tetrahedrons, A_{1g} mode). This was done with the basic objective to investigate, and distinguish between, potential disturbing effects of the chemical composition and/or structural damage as caused by self-irradiation, on the sample's short-range order. These authors observed that the incorporation of non-formula elements, in particular Th^{4+}, U^{4+}, Ca^{2+} and radiogenic Pb^{2+}, causes FWHM (full width at half maximum) increases and shifts of Raman bands.

In this present study, narrow luminescence emissions of REE (rare earth elements) centres with $4f$ electronic structure, such as the $^2H_{3/2} \rightarrow {}^4I_{9/2}$ emission of Nd^{3+} near 11300 cm^{-1} (885 nm wavelength), were found to show similar band broadening/shifting behaviour. In contrast to Raman spectral changes related to phosphate group-vibrations, however, luminescence spectroscopy of REE (i.e., Nd^{3+}) yields information on the crystal field at the substitutional cation sites. We found that the FWHMs of Nd^{3+}emission bands are much more sensitive to the incorporation of heterovalent ions (i.e., SiO_4^{2-}, Th^{4+}, U^{4+}, Ca^{2+}) than to homovalent substitutions ($Ce^{3+} \rightarrow La^{3+}$, Nd^{3+}, Gd^{3+}, etc.). The spectral shift of Nd^{3+} sublevel bands, known as "chemical" shift, depends on the distortional impact of the total amount of incorporated non-formula elements.

Our results may potentially be used to develop a complementary, luminescence-based calibration for the non-destructive quantification of the chemically-induced structural disorder on a micrometre-range, in particular for minerals where suitable Raman bands are absent (i.e., titanite, pyrochlore).

Ruschel, K; Nasdala, L.; Kronz, A., Hanchar, J.M.; Többens, D.M.; Škoda, R.; Finger F.; Möller, A. (2012) : *A Raman spectroscopic study on the structural disorder of monazite–(Ce)*. Mineralogy and Petrology, **105**:41-55