

# Thursday Evening Poster Sessions, October 25, 2018

## Actinides and Rare Earths Focus Topic

### Room Hall B - Session AC-ThP

#### Actinides and Rare Earths Poster Session

**Moderators:** David Shuh, Lawrence Berkeley National Laboratory, James Tobin, UW Oshkosh

#### AC-ThP1 Upconversion Photoluminescence Efficiency Dependence of Yb ions in Gd<sub>0.91-x</sub>NbO<sub>4</sub>: Yb<sub>x</sub><sup>3+</sup>, Er<sub>0.09</sub>, S.S. Yi, *Seung Gon Lee*, Silla University, Republic of Korea

Gd<sub>(0.91-x)</sub>NbO<sub>4</sub>: Er<sup>3+</sup><sub>0.09</sub>, Yb<sup>3+</sup><sub>x</sub> (x= 0.03, 0.06, 0.09, 0.12 and 0.15) phosphors were synthesized by the facile solid state reaction method. Yb<sup>3+</sup> concentrations were changed from 0.03 to 0.15 mol for the fixed Er<sup>3+</sup> concentration at 0.09 mol. The particle size of phosphors was around 180 ~ 350 nm and shape were angular oval observed by scanning electron microscopy. The crystalline structures of the phosphors were investigated by X-ray diffraction. The photoluminescence emission based on the green emissions near 528 and 551 nm and red emissions near 657 and 675 nm were observed and the highest emission intensity occurred for the sample Yb<sub>0.15</sub>Er<sub>0.09</sub>. Also, under the 980 nm excitation, Er<sup>3+</sup>, Yb<sup>3+</sup> co-doped GdNbO<sub>4</sub> phosphors appeared the up-conversion emission based on the green emission near 535 nm and 556 nm radiated by <sup>2</sup>H<sub>11/2</sub> → <sup>4</sup>I<sub>15/2</sub> and <sup>4</sup>S<sub>3/2</sub> → <sup>4</sup>I<sub>15/2</sub> transitions and red emission about 657 nm and 675 nm radiated by <sup>4</sup>F<sub>9/2</sub> → <sup>4</sup>I<sub>15/2</sub> transition, which assigned to the intra 4f transitions of Er<sup>3+</sup> ions.

#### AC-ThP2 Luminescence Characteristics of (Gd<sub>0.85-x</sub>Yb<sub>0.15</sub>)NbO<sub>4</sub>:Er<sub>x</sub><sup>3+</sup> Phosphors, S.S. Yi, *Donggyu Lee*, Silla University, Republic of Korea

Gd<sub>(0.85-x)</sub>NbO<sub>4</sub>: Yb<sup>3+</sup><sub>0.15</sub>, Er<sup>3+</sup><sub>x</sub> (x= 0.03, 0.06, 0.09, 0.12 and 0.15) phosphors were synthesized by the solid state reaction method. Er<sup>3+</sup> concentrations were changed from 0.03 to 0.15 mol for the fixed Yb<sup>3+</sup> concentration at 0.15 mol. The crystalline structures of the phosphors were investigated by X-ray diffraction. The particle size of phosphors was around 140 ~ 320 nm and shape were angular oval observed by scanning electron microscopy. The photoluminescence emission based on the blue emission near 471 nm, green emission near 596 nm and red emission near 621 nm were observed and the highest emission intensity occurred for the sample Yb<sub>0.15</sub>Er<sub>0.09</sub>. Also, under the 980 nm excitation, Er<sup>3+</sup>, Yb<sup>3+</sup> co-doped GdNbO<sub>4</sub> phosphors appeared the up-conversion emission based on the green emission near 535 nm and 556 nm radiated by <sup>2</sup>H<sub>11/2</sub> → <sup>4</sup>I<sub>15/2</sub> and <sup>4</sup>S<sub>3/2</sub> → <sup>4</sup>I<sub>15/2</sub> transitions and red emission about 657 nm and 675 nm radiated by <sup>4</sup>F<sub>9/2</sub> → <sup>4</sup>I<sub>15/2</sub> transition, which assigned to the intra 4f transitions of Er<sup>3+</sup> ions.

#### AC-ThP3 Exploring the Electronic Structure of Molecular Lanthanide Complexes in the +2 Oxidation State Using Photoelectron Spectroscopy, *Daniel Huh, J.P. Bruce, J.C. Hemminger, W. Evans*, University of California, Irvine

Recent advances in rare-earth metal reduction chemistry have led to the isolation of a new series of Ln(II) complexes. For Ln = Y, La, Ce, Nd, Gd, Tb, Dy, Ho, Er, and Lu, reduction of 4f<sup>n</sup> (C<sub>5</sub>H<sub>4</sub>SiMe<sub>3</sub>)<sub>3</sub>Ln<sup>III</sup> complexes generates [(C<sub>5</sub>H<sub>4</sub>SiMe<sub>3</sub>)<sub>3</sub>Ln<sup>II</sup>]<sup>2+</sup> products that exhibit unusual 4f<sup>n</sup>5d<sup>1</sup> mixed-principal quantum number electron configurations. X-ray photoelectron spectroscopy (XPS) has been employed to examine and compare these mixed-principal quantum number electronic structures with those of traditional Ln(II) complexes that have 4f<sup>n+1</sup> configurations. In this work, X-ray and ultraviolet photoelectron spectroscopy have been used to examine the electronic structure of [K(2.2.2-cryptand)][(C<sub>5</sub>H<sub>4</sub>SiMe<sub>3</sub>)<sub>3</sub>Ln<sup>II</sup>] (Ln = Eu, Gd, Tb) where Gd(II) and Tb(II) have previously been shown to have non-traditional 4f<sup>7</sup>5d<sup>1</sup> and 4f<sup>8</sup>5d<sup>1</sup> electronic configurations, respectively, and where Eu(II) has been shown to have a traditional 4f<sup>7</sup> electronic configuration.

#### AC-ThP5 Magnetism of the (Nd,R)<sub>2</sub>Fe<sub>14</sub>B - H system with R = Er and Tm, *I. Tereshina, Lev Ivanov*, M.V. Lomonosov Moscow State University, Russian Federation; *D. Gorbunov*, Helmholtz-Zentrum Dresden-Rossendorf, Germany; *M. Paukov*, Charles University, Prague, Czech Republic; *E.A. Tereshina-Chitrova*, Institute of Physics, Academy of Sciences of the Czech Republic; *M. Doerr*, Technische Universität Dresden, Germany; *L. Havela*, Charles University, Prague, Czech Republic; *A.V. Andreev*, Institute of Physics ASCR, Czech Republic

Since the discovery in 1984, the R<sub>2</sub>Fe<sub>14</sub>B (R is a rare earth) compounds received a considerable scientific attention due to their hard magnetic properties [1,2]. Fundamental characteristics of the best permanent magnet Nd<sub>2</sub>Fe<sub>14</sub>B are known to be highly sensitive to the atomic

substitutions and absorbed light atoms such as hydrogen. In the present work, we studied a combined influence of substitutions of Er and Tm for Nd and hydrogen absorption on the behavior of magnetization in magnetic fields up to 60 T. All studies were conducted on free powder samples at 2 K.

It is found that the substitution in the rare earth sublattice decreases the saturation magnetization as a result of ferrimagnetic ordering of magnetic moments of heavy rare earths with respect to the moments of Nd and Fe. However, under sufficiently strong magnetic fields the magnetic moments rotate and in the ideal case, the field-induced ferromagnetic state is observed. This phenomenon is directly connected to the strength of the inter-sublattice exchange interactions (Fe and Nd, Er, Tm sublattices).

In the parent materials (Nd<sub>0.5</sub>Er<sub>0.5</sub>)<sub>2</sub>Fe<sub>14</sub>B and (Nd<sub>0.5</sub>Tm<sub>0.5</sub>)<sub>2</sub>Fe<sub>14</sub>B in fields up to 60 T no increase of the magnetization was observed. Hydriding of the compounds up to the maximum possible hydrogen content 5.5 at.H/f.u. allows us to observe a forced-ferromagnetic state in the (Nd<sub>0.5</sub>Tm<sub>0.5</sub>)<sub>2</sub>Fe<sub>14</sub>BH<sub>5.5</sub> compound. The transition from ferri- to the ferromagnetic state occurs gradually: it begins at the 35 T field and finishes at 55 T. For the compound (Nd<sub>0.5</sub>Er<sub>0.5</sub>)<sub>2</sub>Fe<sub>14</sub>BH<sub>5.5</sub> we also observe a magnetization increase. So that, hydrogenation is found to weaken the intersublattice exchange interaction in these three-sublattice materials.

This work is performed with financial support of the grant of Russian Scientific Foundation (project № 18-13-00135). We acknowledge the support of HLD at HZDR (member of the European Magnetic Field Laboratory) and the Materials Growth and Measurement Laboratory (<https://mgml.eu> [<https://mgml.eu/>]).

[1] J. F. Herbst, Rev. Mod. Phys. 63, 819 (1991).

[2] O. Gutfleisch et al. Advanced Mater. 23 (7), 821 (2011).

## Author Index

**Bold page numbers indicate presenter**

— A —

Andreev, A.V.: AC-ThP5, **1**

— B —

Bruce, J.P.: AC-ThP3, **1**

— D —

Doerr, M.: AC-ThP5, **1**

— E —

Evans, W.: AC-ThP3, **1**

— G —

Gorbunov, D.: AC-ThP5, **1**

— H —

Havela, L.: AC-ThP5, **1**

Hemminger, J.C.: AC-ThP3, **1**

Huh, D.: AC-ThP3, **1**

— I —

Ivanov, L.: AC-ThP5, **1**

— L —

Lee, D.G.: AC-ThP2, **1**

Lee, S.G.: AC-ThP1, **1**

— P —

Paukov, M.: AC-ThP5, **1**

— T —

Tereshina, I.: AC-ThP5, **1**

Tereshina-Chitrova, E.A.: AC-ThP5, **1**

— Y —

Yi, S.S.: AC-ThP1, **1**; AC-ThP2, **1**