

by resonant ultrasound spectroscopy [1,2]. The different chemical compositions of the investigated crystals allow for a systematic study of the influence of the Li, Na and Fe content on elastic and piezoelectric properties of tourmalines.

On first heating four samples showed an unexpected irreversible softening of all resonance frequencies. These anomalies are most likely related to an increase of configurational entropy caused by order/disorder processes on certain cation sites. The onset temperature of the softening depends on chemical composition.

The well reproducible spectra collected in the second and subsequent heating/cooling cycles were used for the calculation of elastic and piezoelectric constants and of their temperature derivatives. Both elastic and piezoelectric constants behave almost linearly in the investigated temperature interval. Size and anisotropy of the electromechanical properties are closely related to chemical composition and structural features, respectively.

[1] Migliori A. and Sarrao J., *Resonant ultrasound spectroscopy* (John Wiley & Sons, New York), 1997. [2] Schreuer J., *IEEE Transactions on UFFC*, 2002, 49, 1474.

**Keywords:** tourmaline, order/disorder transition, elasticity

#### FA2-MS16-P16

**Synthesis and characterization of Indium– borate glass-ceramics containing  $\text{Ho}_{0.01}\text{Ce}_{0.74}\text{Zr}_{0.25}\text{O}_{1.995}$  nanorods via incorporation method.** Alemi Abdolali<sup>1\*</sup>, Ali Akbar Khandar<sup>a</sup>, Amin Salem<sup>b</sup>, Leila Kafi –Ahmadi<sup>c</sup>. <sup>a</sup>*Department of Inorganic Chemistry, Faculty of Chemistry, University of Tabriz, Tabriz, IRAN.* <sup>b</sup>*Chemical Engineering Department, Sahand University of Technology, Tabriz, Iran.*  
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Glass ceramics materials are polycrystalline solids containing nanometers to micrometers size crystals embedded in a residual glass matrix[1]. Glass ceramics derive particular interest for several end applications, such as thermal, chemical, biological and dielectric ones, because these systems provide great possibilities to manipulate their properties, such as transparency, strength, resistance to abrasion and coefficient of thermal expansion by selecting the suitable constituent oxides[2]. The purpose of this work was synthesis of Indium–borate glass-ceramics containing  $\text{Ho}_{0.01}\text{Ce}_{0.74}\text{Zr}_{0.25}\text{O}_{1.995}$  nanocrystals with "incorporation method" and characterization with XRD, FT-IR, SEM and DTA analysis. Glasses in the system  $\text{In}_2\text{O}_3$ – $\text{Na}_2\text{B}_4\text{O}_7$  were fabricated via melt quenching technique. The amorphous nature of the quenched glasses was confirmed by X-ray powder diffraction studies. The infrared spectra of the glasses show no boroxol ring formation in the structure of these glasses. A cerium–zirconium mixed oxides ( $\text{Ce}_{0.75}\text{Zr}_{0.25}\text{O}_2$  and  $\text{Ho}_{0.01}\text{Ce}_{0.74}\text{Zr}_{0.25}\text{O}_{1.995}$ ) were obtained by solid-state method. Glass powder and  $\text{Ho}_{0.01}\text{Ce}_{0.74}\text{Zr}_{0.25}\text{O}_{1.995}$  were mixed. The mixture was heated in a crucible. The glass-ceramic sample was obtained by pouring the melts on stainless steel. Obtained samples were annealed at 450°C for 1h to remove thermal strain. DTA analysis of the glass and glass-ceramic samples show an endotherm corresponding to the glass transition and an exotherm corresponding crystallization temperature. The difference between  $T_g$  and  $T_x$  (i.e.  $\Delta T = T_x - T_g$ ) in curves DTA is larger for the  $\text{Ho}_{0.01}\text{Ce}_{0.74}\text{Zr}_{0.25}\text{O}_{1.995}$  containing specimen, indicating that the thermal stability of glass-ceramic is higher than that of the glass without crystal. The scanning electron microscopy study for glass-ceramic indicates that the crystallized glass consists of rod-like

crystals with average diameter of about 38 nm dispersed in the glassy regions.

[1] A. Arora, A. Goel, E.R. Shaaban, K. Singh, O.P. Pandey, J.M.F. Ferreir, *Physica B* 403(2008) 173. [2] K. Cheng, *J. Phys. Chem. B* 103(1999) 8272.

**Keyword :** Borate, Glass ceramic, Incorporation

#### FA2-MS16-P17

**Crystal chemistry of silicofluorides.** Tonci Balić-Zunic<sup>a</sup>, Anna Garavelli<sup>b</sup>, Donatella Mitolo<sup>b</sup>, Pasquale Acquafredda<sup>b</sup>, Erik Leonardsen<sup>c</sup>, Sveinn Peter Jakobsson<sup>d</sup>. <sup>a</sup>*Natural History Museum, University of Copenhagen, Denmark.* <sup>b</sup>*Dipartimento Geomineralogico, University of Bari, Italy.* <sup>c</sup>*St. Karlsmindevej 46, Hundested, Denmark.* <sup>d</sup>*Icelandic Institute of Natural History, Reykjavik, Iceland.*  
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The family of silicofluorides includes compounds of alkaline metals or ammonium with silicium and fluorine. Their common structural characteristic is the presence of isolated  $[\text{SiF}_6]$  octahedra. There is a major difference between the coordination of sodium compared with that of potassium and ammonium. As a result, the crystal structure of malladrite ( $\text{Na}_2\text{SiF}_6$ ) [1][2] is significantly different from those of potassium or ammonium compounds. In malladrite fluorine atoms form a hexagonal eutaxy. In this arrangement half of vacant octahedrally-coordinated  $\text{XF}_6$  sites are occupied in ratio 1 $\text{SiF}_6$ :2 $\text{NaF}_6$ . On the contrary, the structures of potassium or ammonium silicofluorides are based on eutactic arrangements where both fluorine and potassium/ammonium partake and silicon atoms fill isolated octahedral holes surrounded exclusively by fluorine atoms. Structures with both cubic-eutaxy and hexagonal-eutaxy stackings can be found in this part of the family, as well as with a special ...ABCBABC... stacking of layers. In the structure of the new mineral heklaite ( $\text{KNaSiF}_6$ ) [3][4] the eutactic arrangement of fluorine and Na/K atoms is not present, due to distortion of K coordination. It is a peculiarity of this structure that the cation with shorter bond lengths (Na) has a larger coordination number (10) than the cation with the longer bond lengths (K; CN 9) [3]. The fundamental differences between the Na and K coordinations in heklaite, plus the difference between its structure and those of  $\text{Na}_2\text{SiF}_6$  and  $\text{K}_2\text{SiF}_6$  polymorphs suggest absence of solid solution in the pseudo-binary phase field  $\text{Na}_2\text{SiF}_6$ - $\text{K}_2\text{SiF}_6$  which is confirmed by the field observations on the type locality for this mineral, Hekla volcano on Iceland [4].

[1] Zahlkin A., Forrester J.D., Tempelton D.H. *Acta Cryst.*, 1964, 17, 1408. [2] Schäfer G.F. *Zeitschrift Krist.*, 1986, 175, 269. [3] Fischer J., Krämer V. *Mat. Res. Bulletin*, 1991, 26, 925. [4] Garavelli A., Balić-Zunic T., Mitolo D., Acquafredda P., Leonardsen E., Jakobsson S.P. *Min. Mag.*, in print.

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#### FA2-MS16-P18

**Metamict Titanite.** Tobias Beirau, Ulrich Bismayer, Carsten Paulmann. *Universität Hamburg, Germany.*  
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The structure of the pure mineral titanite with chemical composition  $\text{CaTiSiO}_5$  consists of corner linked  $\text{TiO}_6$ -octahedra,  $\text{SiO}_4$ -tetrahedra and sevenfold coordinated Ca