Poster Session

⁵⁷Fe Mossbauer spectroscopy study of the Fe-bearing, Ge,Ga-rich synthetic tourmalines

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Borosilicate mineral tourmaline is one of the most widespread minerals in nature, one of the most popular gems and promising piezoelectric, adsorption material [1,2]. Synthetic Ga,Ge-rich analogue is structure model of tourmalines at high pressure. This work presents the results of Mössbauer studies of Ga,Ge-rich tourmaline crystals which contain a significant iron content. The crystals were grown in hydrothermal boric, boric-alkaline, boric-fluoride solutions at 650 °C and 100 MPa [3,4]. The chemical composition of the five studied tourmaline crystals in atoms per formula unit, calculated based on the 15 (T + Y + Z) atoms, is shown in Table 1.

№	Si	Ge	Al	Fe	Ga	Ni	Ti	Ca	Na
60/8	5.61	1.16	5.75	2.00	1.06	0.26	0.16	0.00	0.46
60/7	4.86	0.81	6.11	1.89	1.23	0.03	0.07	0.00	0.47
60/5	5.48	0.22	7.46	1.06	0.73	0.05	0.00	0.04	0.05
59/26	5.44	0.21	5.46	1.26	2.56	0.00	0.07	0.05	0.61
63/6	5.51	0.55	6.94	1.58	0.57	0.19	0.00	0.00	0.00

Table 1

The ⁵⁷Fe Mössbauer absorption spectra were measured at room temperature on a standard MS-1104Em spectrometer with a ⁵⁷Co (Rh) source. The structural and electronic states of iron ions have been studied and refined. A comparison is made with the results of X-ray diffraction measurements.

- [1] Wang, C. P.; Wu, J. Z.; Sun, H. W.; Wang, T.; Liu, H. B.; Chang, Y. Adsorption of Pb(II) Ion from Aqueous Solutions by Tourmaline as a Novel Adsorbent. Ind. Eng. Chem. Res. 2011, 50 (14), 8515–8523. https://doi.org/10.1021/ie102520w.
- [2] Shekhar Pandey, C.; Schreuer, J. Elastic and Piezoelectric Constants of Tourmaline Single Crystals at Non-Ambient Temperatures Determined by Resonant Ultrasound Spectroscopy. J. Appl. Phys. 2012, 111 (1). https://doi.org/10.1063/1.3673820.
- [3] Setkova, T. V.; Balitsky, V. S.; Shapovalov, Y. B. Experimental Study of the Stability and Synthesis of the Tournaline Supergroup Minerals. Geochemistry Int. 2019, 57 (10), 1082–1094. https://doi.org/10.1134/S0016702919100094.
- [4] Pushcharovsky, D. Y.; Zubkova, N. V.; Setkova, T. V.; Balitskii, V. S.; Nekrasov, A. N.; Nesterova, V. A. (Ga,Ge)-Analogue of Tourmaline: Crystal Structure and Composition. Crystallogr. Reports 2020, 65 (6), 849–856. https://doi.org/10.1134/S1063774520060279.

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