

**[o.m13.p21] Admixtures in Synthetic Zircons: SEM and XRD Study.** A. Maslenikov, J. Plotkina. *Institute of Precambrian Geology and Geochronology Rus. Acad. Sci., Makarova Emb. 2, St-Petersburg 199034 Russia.*  
Keywords: zircon, admixture, structure.

Synthetic zircon crystals with admixture of  $V^{4+}$ ,  $Cr^{3+}$ ,  $Nb^{4+}$ ,  $Nd^{3+}$ ,  $W^{6+}$ ,  $Ta^{5+}$  cations (up to 1 wt.%) were investigated by SEM and XRD methods.

These crystals are prismatic, idiomorphic, optically homogeneous and without visible growth zoning. The surface morphology is equal for crystals with admixtures and without ones (Fig. 1a, b).

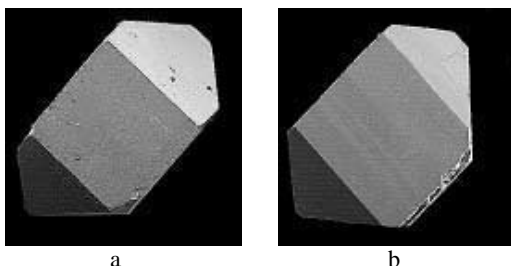


Fig. 1. SEM (ABT-55) image of zircon crystals:  
a - without admixtures;  
b - with 0.5 wt. %  $Nb^{4+}$ .

The high degree of crystallinity is the characteristic of the samples. Unit-cell parameters (powder diffraction X-ray method,  $CoK\alpha$ , 9-12 reflections)  $a=6.600(1)A$  and  $c=5.976(1)A$  are constant for all samples.

The absence of visible morphological and structural differences of studied samples can be explained by small amount of admixtures.

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**[o.m13.p22] Tellurium crystal chemistry in some new tellurite compounds.** J.C. Champarnaud-Mesjard, P. Thomas, S. Blanchandin, M. Dutreilh, B. Frit., *SPCTS, UMR CNRS 6638, Faculté des Sciences, 123 Avenue Albert Thomas, 87060 Limoges Cedex, France.*  
Keywords: tellurite, crystal structure, X-ray diffraction.

Numerous recent studies have shown that  $TeO_2$ -based glasses are interesting materials for non-linear optical applications. The origin of such exceptional properties was clearly attributed to the hyperpolarizability of the  $Te^{IV}$  atoms lone pair which is very often reinforced by addition of a second lone pair holder (such as  $Bi^{3+}$ ,  $Pb^{2+}$ ,  $Tl^+$ ) and/or cations with empty d-orbitals (such as  $W^{6+}$ ,  $Nb^{5+}$ ,  $Ti^{4+}$ ). In such glasses, it has been shown that additions of oxides of mono-, di-, tri-, and tetravalent cations to  $TeO_2$  leads to a continuous transformation of trigonal bipyramidal  $TeO_4E$  units into tetrahedral  $TeO_3E$  units via  $TeO_{3+1}$  units (E: lone pair of  $Te(IV)$  atoms). The non-linear properties of these glasses are strongly related to their structure whose knowledge is therefore of prime importance. The structure of tellurite glasses is so of great interest. From this point of view, we have investigated within the  $TeO_2$ - $Tl_2O$ - $Bi_2O_3$ ,  $TeO_2$ - $Nb_2O_5$ - $Bi_2O_3$  and  $TeO_2$ - $Tl_2O$ - $Ga_2O_3$  systems. Considering that the knowledge of the crystal structure of the stable or metastable phases which could appear during the crystallisation of such glasses should give us precious informations about the short range order in the corresponding glasses, we have undertaken a systematic structural study of them using single crystal or powder X-ray diffraction. We will present in this communication the crystallochemical behaviour of the  $Te(IV)$  atoms in some metastable or stable tellurite compounds such as  $\delta$ - $TeO_2$ ,  $\gamma$ - $TeO_2$ ,  $\beta$ - $TeO_2$  [1],  $\alpha$ - $TeO_2$  [2],  $Tl_2TeO_3$ ,  $\alpha$ - $Tl_2Te_2O_5$ ,  $Tl_2Te_3O_7$ ,  $Nb_2Te_4O_{13}$ ,  $BiNbTe_2O_8$ ,  $Ga_2Te_4O_{11}$ . For example, for thallium tellurite compounds we have shown that from  $TeO_2$  to  $Tl_2TeO_3$  the anionic coordination polyhedron of  $Te^{4+}$  changes progressively from a  $TeO_4$  disphenoid to a  $TeO_3$  trigonal pyramid via an intermediate  $TeO_{3+1}$  polyhedron. The anionic polyhedra of  $Tl^+$  cations show nearly the same kind of evolution with a progressive transformation of the  $TlO_4E$  trigonal bipyramids, observed in  $Tl_2Te_3O_7$ , into the perfect  $TlO_3E$  tetrahedra of  $Tl_2O$ . Such evolutions clearly indicate that increasing thallium content enhances the anisotropic character of the anionic arrangement around cations and that the stereochemical activity of the lone pair of  $Te$  atoms is strengthened by the presence of a second lone pair holder.

[1] H.Beyer, "Verfeinerung der Kristallstruktur von Tellurit, dem rhombischen  $TeO_2$ ", *Zeitschrift für Kristallographie*, (1967), 124: 228-237.

[2] P.A.Thomas, "The crystal structure and absolute optical chirality of paratellurite,  $\alpha$ - $TeO_2$ ", *J. Phys. C: Solid State Phys.*, (1988), 21: 4611-4627.