

Ti-investigation by xps OF biotite From Metapelites of El Joyazo (Spain)

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The Ti-rich biotite from graphite-bearing metapelitic xenoliths (El Joyazo – Spain) have been recently studied through a multitechnical approach [1]. The study, combining several techniques, showed TiO₂ content ranging from 4.5 to 4.9 wt% and a constant X_{Fe} = 0.67. According to the results of their investigations, Cesare *et al.* [1], suggest that titanium (as Ti⁴⁺) is logged only in octahedral site. The aim of the present work is the investigation both the oxidation state and the site partition of titanium accepting the main crystal chemical conclusion achieved by [1]. The following Ti-coordination polyhedra have been considered during XPS analysis: 4-fold coordination (tetrahedral), 5+1 coordination (distorted octahedral), 6-fold coordination (regular octahedral). In order to obtain the best fitting, the BE of the Ti⁴⁺ for the octahedral and tetrahedral coordination have been determined following the procedure in [2]. While the BE for Ti⁴⁺ in distorted octahedron (5+1) has been obtained by means of *ab initio* calculations [3]. The result of XPS investigation shows that Ti⁴⁺ populates both tetrahedral and octahedral sites. Taking in account the structural formula proposed by [1], we note that the entrance of Ti⁴⁺ in the tetrahedral site and of Al³⁺ in octahedral site, in the same amount, results in a both better balance of the substitution mechanisms and in a better m. a. n.'s agreement between EPMA and SCXRD data.

[1] Cesare B., Cruciani G., Russo U., *Am. Mineral.*, 2003, **88**, 583-595. [2] Malitesta C., Losito I., Scordari F., Schingaro E., *Eur. J. Mineral.*, 1995, **7**, 847–858. [3] Saunders V.R. *et al.*, *CRYSTAL'03 User Manual*, Turin, University of Torino, 1999.

Keywords: Ti-bearing micas, XPS analysis, Ti speciation