Analysis of vacant positions in the structure of pyrite

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Pyrite (FeS_2) almost always has not a stoichiometric composition, and therefore has cationic and anionic vacant positions in the structure. The composition of natural pyrite better represent the by the chemical formula $(Fe^{+2})_{\alpha}((S_2)^{-2})_{\beta}$. If α and β are equal 1 (stoichiometric composition), iron in the sample shall be 46.55 wt. %, and sulfur - 53.45 wt. %. Only in this case the structure of pyrite no cationic or anionic vacancies. Thus, S/Fe relation in that case can be defined with a bigger accuracy from the relation $2\beta/\alpha$ as each position of a dumbbell is taken by two atoms of sulfur, and density of vacant positions (n) will be defined by the equation: $(1 - \alpha) = (2\beta - 2) = n$. Was investigated area of pyrite "Panimba" deposits (Krasnoyarsk region, Russia). The chemical composition of the samples in the laboratory of microprobe analysis (EPMA) was determined.

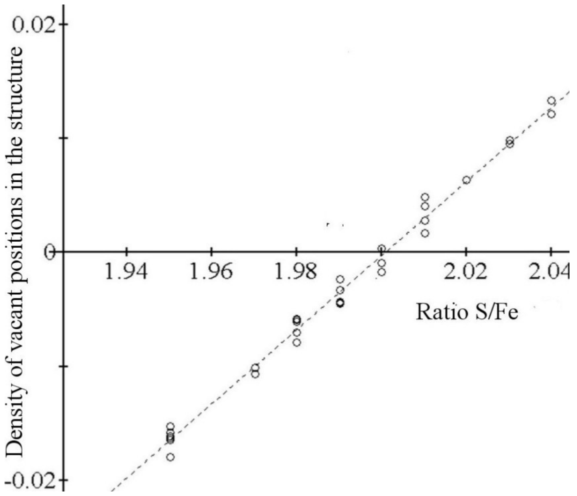

Fig.1. Density vacant positions in the structure of pyrite with different ratios S/Fe.

The curve in fig. 1 shows that the samples with the same value of S/Fe may have a different density of vacancies in the structure. Shown that the ratio S/Fe = 2.00 in pyrite is not a necessary and sufficient condition for the absence of vacant positions in the structure. More important, in this sense, is not the ratio S/Fe, but the percentage of Sulfur and Iron in the samples.