Analysis of point defects in the structure of chalcopyrite

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Chalcopyrite is almost always a non-stoichiometric. Given the presence of the impurity atoms in the structure of chalcopyrite should clarify the formula: $(Fe)_{\alpha}(Z)_{\varrho}(Cu)_{\varkappa}(S_2)_{\beta}$, where Z may represent impurity atom, e.g., Co, Ni, Au and Zn. The ratio A(anion)/C(cation) in this case is the ratio of $2\beta/(\alpha+\varkappa)$, because each anionic vacant position corresponds to two sulfur atoms, consequently, the density vacant positions (n) is defined by the equation: $n = \beta-(\alpha+\varkappa)/2$.

If α, $\varkappa$ and β are equal to unity (stoichiometric composition $CuFeS_2$), then, as the calculation of iron in the sample shall be 30.43 wt. %, copper - 34.63 wt. % , sulfur - 34.94 wt. %. Only in this case the structure of chalcopyrite no cationic or anionic vacancies. Analysis of allows to make a conclusion that the total density of the impurity atoms is practically independent of the ratio S/(Fe + Cu) in the samples. Was investigated chalcopyrite from "Panimba" deposits (Krasnoyarsk region, Russia). The chemical composition of chalcopyrite was determined in the laboratory of microprobe analysis (EPMA) in Novosibirsk- city.

A/C	$n \cdot 10^{-2}$	$\varrho_{Co} \cdot 10^{-2}$	Co;wt.%	$\varrho_{Au} \cdot 10^{-3}$	Au;wt.%
0.988	-1,187	0,113	0.044	0.023	0.003
0.994	-0.623	0.111	0,043	0,085	0.011
0.999	-0.120	0.067	0.026	0.062	0.008
1.001	0.055	0.095	0.037	0.177	0.023
1.007	0.655	0.036	0.014	0.162	0.021
1,012	1.156	0.072	0.028	0.215	0.028

Table 1. Selected results EPMA and calculations (ϱ_{Co}, ϱ_{Au} and n) only for impurity atom of Co and Au.

The unit cell of chalcopyrite corresponds to the structure of the superstructure of sphalerite, as formed by two cell types sphalerite, put on each other along the axis of the "c". In such a structure should be free octahedral sites, and they occupy the impurity atoms. These positions do not depend on the density vacant positions in the parent matrix.

In the structure of samples even with equal density of vacancies, the density of the impurity atoms subject to change in magnitude. If there is no vacant positions in the structure analysis of the results shows that the presence of impurities in structure possibly.