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Some Comments on Pyrite's Structure

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ABSTRACT

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Introduction

Pyrite, a natural mineral with chemical formula of FeS_2, is widely distributed in ores [1,2]. Relatively high concentration of impurity atoms in pyrite is obviously reflects its mineral typomorphism. One of the factors, influencing the typomorphic properties of minerals, is presence of vacancies in their crystal structures [3,4]. The conditions of pyrite's formation vary. It is widespread in hydrothermal ore veins; a broad temperature interval is typical of the processes of its formation. Pyrite may be found in high-temperature post-magmatic (pneumalitic) deposits, sometimes in zones of the contact metamorphism. Moreover, magmatic processes also give birth to small amount of the mineral [5-10]. The impurity atoms of metals may occupy:

a) Positions of cationic vacancies,

b) Interstitial positions (of crystal lattice), or

c) Isomprphically subsitute ions of the basic matrix, situated at lattice points. Actuality of researching impurity atoms in each of the three possible positions in the crystal structure is clear because different admixture inclusions may shape a mineral's properties in their own ways.

For instance, impurity atoms, located at lattice points, deform a crystal structure of the basic structural matrix. The influence of structural deformations may become, in some cases, crucial in the process of studying the influence of certain factors upon mineral characteristics [5,4]. For instance, almost all particles of iron sulfides with the size of 80 Å or less have structural distortions (as a result of the relatively high superficial energy). This may be reflected in a number of these specimens' specific magnetic properties [10,11]. In the case of isomorphic substitution pyrite transforms – depending on a kind of impurity atoms - into other minerals. For example, if pyrite contains Cu, Ni, Co or Fe atoms, such minerals may emerge as villamanite (Cu,Ni,Co,Fe)S2, bravoite $(Fe,Ni)S_2$, or, if iron atoms are totally replaced by ones of nickel and cobalt, vaesite NiS_2 and cattierite CoS_2. All these minerals create an isostructural group, the Pa3 space group. In the case of total isomorphic substitution, the minerals of pyrite's group are to be represented as AX2, where A is such a chemical element as Au, Co, Cu, Fe, Mn, Ni, Os, Pd, Pt, or Ru. X of the formula is As, Bi, S, Sb, Se, or Te. The "A" atoms occupy the points of a face-centered cubic lattice and are surrounded by the dumb-bell coupled "X" atoms [10].

The influence of an impurity atoms' structural substitution type upon properties of minerals is studied fragmentarily; therefore, the impurity atoms' positions in the pyrite structure need further investigations. It is necessary to find a criterion tied to the way of entering ones or other impurity atoms into the crystal structure as soon as its properties in many respects are predefined by a character of this penetration. The work [1] describes a pyrite having the structure distorted so that its crystals are of triclinic system. The reason of the deformation lies in certain conditions of pyrite's formation, not of isomorphic substitutions that unable to cause such distortions of pyrite's structure by themselves. It is clear that the positions and intensiveness of X-ray reflexes at such pyrite's diffractogram diverge from the ones at ideally structured pyrite's diffractogram, that are not necessarily related to the isomorphic substitution. The latter may affect a type of conductivity, but the analyzed work [10] for some reason ties changing type of conductivity to the S/Fe ratio in specimens. It is to be stressed in order to show (by a certain example) that, despite the noticeable value of such works' geological components, their analysis of minerals' structure and properties look very questionable. This again confirms the actuality of further studies, focused on structural peculiarities of pyrite as well as their structural transformations at the time of formation or decomposition, influenced by external factors (such as pressure or temperature).

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