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XAS investigation of 'invisible' gold impurities in synthetic sulfide minerals

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Gold in ores of hydrothermal and magmatic origin deposits in the form of its own crystalline phase (usually in the form of an alloy with the silver - electrum) or dispersed in sulfides as isomorphic impurity, nanosized particles Au⁰ or chalcogens and compounds with semimetals (As, Sb, Bi, Te). Scattered ("invisible") form of gold is much more difficult to remove when ore processing, and most part of it becomes waste. To determining the structural and chemical state (degree of oxidation and structural position) of "invisible" gold atoms we synthesized gold minerals systems Cu-S, Fe-S, Cu-Fe-S and Fe-As-S. Synthesized minerals were studied by X-ray spectroscopy at the LIII edge of gold. Measurements were made at ESRF and "Kurchatov synchrotron center". Data treatment were made using computational methods for optimization geometry of gold inclusions in mineral structure (Quantum Espresso) and finite difference method for XAS calculation (FDMNES). EXAFS spectra were measured for several model systems at "Kurchatov synchrotron center". Fitting of EXAFS data has provided information concerning local atomic structure around absorbing Au atoms. HERFD-XANES spectra were collected ID26 beamline at ESRF for several reference samples and minerals with gold inclusions. Comparison with standards and modeling spectra, calculated using FDMNES, showed that in covellite Au atoms incorporated into disulfide groups. This form of "invisible" gold is stable in a wide range of temperatures and does not break during the quenching system. In other minerals of Cu-Fe-S gold is in the form of a solid solution, stable only at high temperatures .

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