Digital recording of XRD spectra for minerals opens new possibilities of using XRD structural characteristics such as full width at half-maximum (FWHM), width of integral reflexes (I. Breadth), position of center of gravity of reflex (Gravity C.) and corresponding d-spacing (Gravity C.), area of reflex (Net Area) for geological exploration – from search and evaluation of mineral resources to rational schemes of enrichment and extraction of valuable components.

For example, XRD study of powder samples of pyrite from important pyrite deposits and some copper-porphyry, gold, lead-zinc, iron ore and rare metal deposits of Kazakhstan has shown informative value of XRD structural characteristics as physicochemical indicators of ore forming. Impurities of typical mineral microinclusions, unit cell parameter, crystalinity and other structural characteristics of pyrite were determined. The variety of physicochemical parameters of pyrite generation has slight impact on unit cell parameter. Conditions of pyritiferous ores formation to a large degree effect on defects of mineral crystal structure, which indicate as changing of reflex shape. Different coefficients and criteria, that used for quantitative estimation of crystalinity, allow to compare obtained factors of pyrite structural state from genetically different deposits, when measuring series of samples in the same mode. Since the intensity distribution in the diffraction profile depends on many factors (microdistortion of the crystal lattice, dispersion of the crystallites, their zoning and inhomogeneity etc.) as a universal quantitative evaluation of crystalinity, we propose to use the FWHM. XRD characteristics of crystalline state of ore and rock-forming minerals delivers a lot of valuable information for geological research. The value of FWHM is advisable to put in Powder Diffraction Files (PDF) of the International Centre for Diffraction Data (ICDD), along with Corundum Number for a specific sample of mineral.


Keywords: Pyrite, crystalinity, FWHM