

TETRAGONAL AND HEXAGONAL POLYMORPHS OF $\text{BaTi}_{1-x}\text{Fe}_x\text{O}_3$ - MULTIFERROICS USING X-RAY AND RAMAN ANALYSES (SCI)

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TÓM TẮT:

The effect of Fe doping on the crystalline phase transformation and on the local environment around Fe dopant ions is investigated for $\text{BaTi}_{1-x}\text{Fe}_x\text{O}_3$ ($0.0 < x < 0.5$) polycrystalline samples, using x-ray diffraction, x-ray absorption spectroscopy, and Raman scattering spectroscopy. Our experimental results show that the tetragonal-to-hexagonal transformation is gradually taken place when increasing the Fe content in the range $0.02 < x < 0.12$. Although both hexagonal and tetragonal polymorphs coexist in this doping range, Fe ions preferably substitute for Ti sites in the hexagonal lattice and exist in both Fe^{3+} and Fe^{4+} forms. Our work is of paramount importance to provide a direct evidence to the preferable substitution of transition metal ions for Ti ions.