

The marcasite-pyrite transformation: the roles of water vapor, trace elements and grain size

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Despite the natural abundance of intergrown pyrite and marcasite, and a wealth of information they provide on the physical-chemical conditions of mineral deposits, a complete mechanistic and kinetic study on the phase transformation from the thermodynamically metastable polymorph marcasite to the stable polymorph pyrite is yet to be made. This limits the application of marcasite as an indicator mineral for low temperature geological environments.

Here we report results from *in situ* synchrotron powder XRD and *ex situ* anneal/quench experiments at 400-540°C, demonstrating that the mechanism and kinetics of this transformation depend not only on temperature, but also on the presence of water vapor, particle size, and the presence of pyrite inclusions in marcasite [1]. For example, under dry conditions, the transformation is controlled by epitaxial growth of pyrite on marcasite, but in the presence of water vapor, epitaxial growth is insignificant. Consequently, the kinetics is very different in dry and water vapor conditions. Synchrotron XRF results suggest that trace elements like As and Pb play insignificant role in the transformation but the transformation affects trace elements redistributions in pyrite. Kinetic analysis estimates a half-life of 1.5 Ma at 300 °C for the transformation under dry conditions with small (38-53 µm) and pyrite-free marcasite grains. However, this estimation should be applied with caution due to the complexity of the transformation.

This study highlights that although the natural occurrence of marcasite can indicate low temperature environments, precise temperature estimation should consider the roles of various factors.

[1] X. Z. Yao, F. Xia, A. P. Deditius, J. Brugger, B. E. Etschmann, M. A. Pearce, A. Pring, *Contributions to Mineralogy and Petrology*, 2020,
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