ELECTRON MICROSCOPY STUDY OF {110} INTERPENETRATION TWINS OF PYRITE

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Interpenetration twins of pyrite were first described from Weserbergland in Germany. Owing to characteristic crosses coinciding with {100} faces they were named iron-cross twins. Crystallographically, iron-cross twins are produced by 180° rotation about the $[1\,\bar{1}\,0]$-axis, however there is very little known about the actual twin boundary structure at the atomic scale. Based on fringe contrast of a low-resolution TEM image recorded on an inclined twin boundary DONNAY *et al.* (1977) reported that twin boundaries in pyrite are curved extended defects not bound to any of the low-index lattice planes. They proposed an idealized twin boundary model with a continuous Fe-sublattice across (110) interface comprising unit-cell steps alternated between (100) to (010) planes. Although anticipated, no impurity elements could be detected on the twin boundary.

In our study we used twinned pyrite crystals from Mt. Katarina, Slovenia (REČNIK, 2007). The crystal habit is dominated by the pentagon-dodecahedral {210} form, which makes the interpenetration twinning macroscopically visible. Twinned crystals of pyrite were cut parallel to the (001) plane, maintaining the nucleation point of the two intersecting $(\bar{1}\,10)$ and (110) twin planes near the centre of the TEM specimen. A quick glance over the TEM specimen revealed that near the centre of the crystal the boundaries between interpenetrating twin domains generally follow {110} planes and make intermittent steps to {100} planes, whereas in the outer regions {100} interfaces become more and more common, while {110} boundaries gradually cease to exist. Due to the fact that twin boundaries can occupy 6 parallel pairs of {110} planes and 3 parallel pairs of {100} planes where only 2 of each are edge-on, while all other are either inclined or lie in-plane with respect to the selected viewing direction. For this reason, it is quite a challenge to find an area suitable for HRTEM investigations. According to our observations the primary {110} twin boundary (type-A) can deflect into secondary {100} interfaces (type-B), following a simple crystallographic relation: (110) → a·(100) + b·(010), where the fractions of both components are a = b for an idealized interpenetration twin, and a ≠ b in the case of realistic twins. EDS chemical analysis of individual interfaces showed that the primary (type-A) twin boundaries comprise a significant amount of Cu, whereas the secondary (type-B) twin boundaries are devoid of dopants. Using a concentric electron probe (CEP) method (WALTHER *et al.*, 2004) we have shown that 0.18 ± 0.03 nm of the type-A twin boundary is occupied by copper, which with respect to the structural density of pyrite, would correspond to one full monolayer of Cu. While the local atomic structure of {110} and {100} twin boundaries are not yet resolved, present results suggest that these are growth twins, which formation is triggered by the incorporation of Cu in the nucleation stage.

References

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