

The occurrence of P, Al and Si impurities in Australian iron ores: the goethite connection

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Mining and recovery of Fe-oxides underpins Australia's mining sector. Declining production of high-grade hematite ores has led to an increasing reliance on lower grade, impurity-containing goethitic ores. In this study we determine the distribution and association of the critical impurities Al, Si and P within different goethite textural types in Australian iron ores. A detailed characterisation study using XRF and QXRD techniques to provide chemistry and mineralogy followed by hyperspectral EPMA to identify impurity element distributions and textural associations. In element maps a strong association between P, Al and Si was noted and after follow-up quantitative analyses a coupled substitution mechanism for P, Al and Si incorporation within goethite was proposed: $2\text{Si}^{4+} = \text{P}^{5+} + \text{Al}^{3+}$. Quantum mechanical modelling examining coupled Al and P incorporation indicated the most stable configuration was reached when Al^{3+} substituted for Fe^{3+} next to a P-induced vacancy defect. This preliminary result appears to support the coupled substitution model.

While the FEG-EPMA analyses offer preliminary conclusions regarding the possible mechanism(s) of P incorporation in goethite, the results could equally be explained by the presence of nanometre size inclusions of P-, Al- and Si-rich phases or adsorbed species such as $[\text{AlPO}_3]^{3+}$. If present, these would be below the ~150 nm analytical resolution of the FEG-EPMA technique and when probed, would appear to be present as solid solution components. To determine conclusively the mechanism of P, Al and Si incorporation requires examination of goethite-rich regions that are known to contain these impurities, via an imaging technique such as high-resolution SEM or a structural identification method such as TEM.

The exact type of substitution mechanism will have important implications in designing strategies for removing impurities from goethitic ores containing high levels of impurities.