The Crystal Structures of the Iron Carbides

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Various low temperature iron carbides are formed in the reactor during the Sasol Synthol process to produce hydrocarbons. The small particle sizes of the iron carbides prevented complete structure determination in the past. Modern equipment is available to study the crystal structures of the iron carbides. The improved crystal structures can then be used to characterize the commercial catalyst samples.

Hägg carbide (χ-Fe_5C_2) and pseudo hexagonal (ε'-$Fe_{2.2}C$) iron carbide samples have been prepared from spray-dried hematite. The preparations were done in an Anton Paar reaction chamber mounted on an X'Pert Pro diffractometer.

The samples were characterized using SEM, powder X-ray diffraction and room temperature Mössbauer spectroscopy. Structure determination with powder diffraction (SDPD) was used to determine the structures of the iron carbides. Rietveld refinements with X'Pert Plus and GSAS software were done on the powder X-ray diffractograms.

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