
Determination of Mean Crystallite Dimensions from X-Ray Diffraction Peak Profiles: A Comparative Analysis of Synthetic Hematites

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Abstract: X-ray diffraction (XRD) profile analysis of eight synthetic hematite samples was performed to identify the best parameters for determining the apparent mean crystallite dimension (D) and, consequently, surface area. The samples are comparable to soil hematite with respect to crystallinity. The procedure included: a) deconvolution of the XRD peaks to Gauss and Cauchy components and subtraction of the instrumental profile, b) determination of D from full-width at half-maximum, integral breadth, and integral breadth measurements of the Cauchy component, and c) comparison of deduced surface areas with those obtained by the N₂-BET adsorption method. As expected, D values are strongly influenced by the broadening parameters. An appropriate selection of peaks is required to obtain size values along the crystallographic axes a (hkl : 110, 300) and c (hkl : 104, 116) and to calculate reliable surface areas. Using the Cauchy component of the above peaks, the calculated surface areas compared well with those measured by the N₂-BET adsorption method.

Key Words: BET • Hematite • Iron Oxides • Mean Crystallite Dimension • Powder X-ray Diffraction • Surface Area • XRD

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