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XRD measurement of mean crystallite thickness of illite and illite/smectite; reappraisal of the Kubler index and the Scherrer equation

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The standard form of the Scherrer equation, which has been used to calculate the mean thickness of the coherent scattering domain (CSD) of illite crystals from X-ray diffraction (XRD) full width data at half maximum (FWHM) intensity, employs a constant, K_{sh}, of 0.89. Use of this constant is unjustified, even if swelling has no effect on peak broadening, because this constant is valid only if all CSDs have a single thickness. For different thickness distributions, the Scherrer "constant" has very different values. Analysis of fundamental particle thickness data (transmission electron microscopy, TEM) for samples of authigenic illite and illite/smectite from diagenetically altered pyroclastics and filamentous illites from sandstones reveals a unique family of lognormal thickness distributions for these clays. Experimental relations between the distributions' lognormal parameters and mean thicknesses are established. These relations then are used to calculate the mean thickness of CSDs for illitic samples from XRD FWHM, or from integral XRD peak widths (integrated intensity/maximum intensity). For mixed-layer illite/smectite, the measured thickness of the CSD corresponds to the mean thickness of the mixed-layer crystal. Using this measurement, the mean thickness of the fundamental particles that compose the mixed-layer crystals can be calculated after XRD determination of percent smectitic interlayers. The effect of mixed layering (swelling) on XRD peak width for these samples is eliminated by using the 003 reflection for glycolated samples, and the 001, 002 or 003 reflection for dehydrated, K-saturated samples. If this technique is applied to the 001