UC DAVIS Chemical Engineering & Materials Science

EMS-162L: Structure and Characterization of Materials Laboratory

Winter Quarter, 2004

Crystallite Size Analysis

1. What is the difference between crystallite size and particle size?

2. The manufacturer's specifications on a nanocrystalline powder states that it has a specific surface area of 48 m^2/g and a density of 5.1 g/cm^3. Assume the particles are spherical and estimate the particle size (diameter).

3. Both the Scherrer and the Warren-Averbach methods measure column lengths for the crystallites. What is meant by the term column length and how does it relate to the size of a crystallite?

4. Your x-ray diffraction analysis of the above powder yields a Scherrer crystallite size (diameter) of 59.2 nm while the Warren-Averbach analysis of the same data yields a crystallite size (diameter) of 26.6 nm. Explain the differences in these two numbers.

5. A series of x-ray diffraction analyses employing both the Scherrer and Warren-Averbach techniques produced the following results.

22	(hkl)	Scherrer Analysis $\langle L \rangle_{Vol}$ (nm)	Warren-Averbach Analysis $\langle L \rangle_{Area}$ (nm)
48.02	(200)	38.5	16.1
107.44	(316)	44.0	18.0
108.93	(400)	50.1	19.2

Using these results:

- Calculate the crystallite sizes (diameters) assuming they are spheres.
- Determine D_0 and F for the log-normal distributions of each reflection and plot these distributions on the same graph. Include data points that show the locations of the three Scherrer and Warren-Averbach sizes.
- Calculate the arithmetic average crystallite size (spheres) for each reflection.
- Compare these three measurements in terms of their size distributions and the arithmetic average crystallite size.