Aufgabe 9-1: ***Williamson – Hall plot***

The X-ray diffraction pattern of the silver nanoparticles synthesized by electrolysis method is shown in Fig. 1. The position and FWHM (full width at half maximum) of the Bragg reflections are given for the Cu kα radiation (λ = 1.54056 Å):

line	2θ of the intense peak (deg)	FWHM of the intense peak (radians)
1	38.3182	0.0041
2	44.4975	0.0048
3	64.6119	0.0038
4	77.5385	0.0034
5	81.6839	0.0038

a) Index the lines and find the corresponding Brava's lattice.

b) Determine the lattice parameter a_0, by graphical extrapolation of "a" against $\cos^2\theta$.

c) Assuming that the major cause of the line broadening is due to the small particle size, estimate the size of the Ag nanoparticles from the *Debye–Scherrer* formula.

$$\beta = \frac{0.9\lambda}{t\cos\theta}$$

Where λ is wave length of X-ray, β is FWHM, θ is the diffraction angle, and t is particle diameter size.

a) The particle size and strain (ϵ) contributions to line broadening can be estimated by *Williamson-Hall* equation:

$$\beta_{hkl}\cos\theta = \frac{0.9\lambda}{t} + 4\,\epsilon\,sin\theta$$

Determine the average particle size t and the strain ϵ of the experimentally observed broadening of the peaks using *least squares method* (instrumental broadening is not considered).

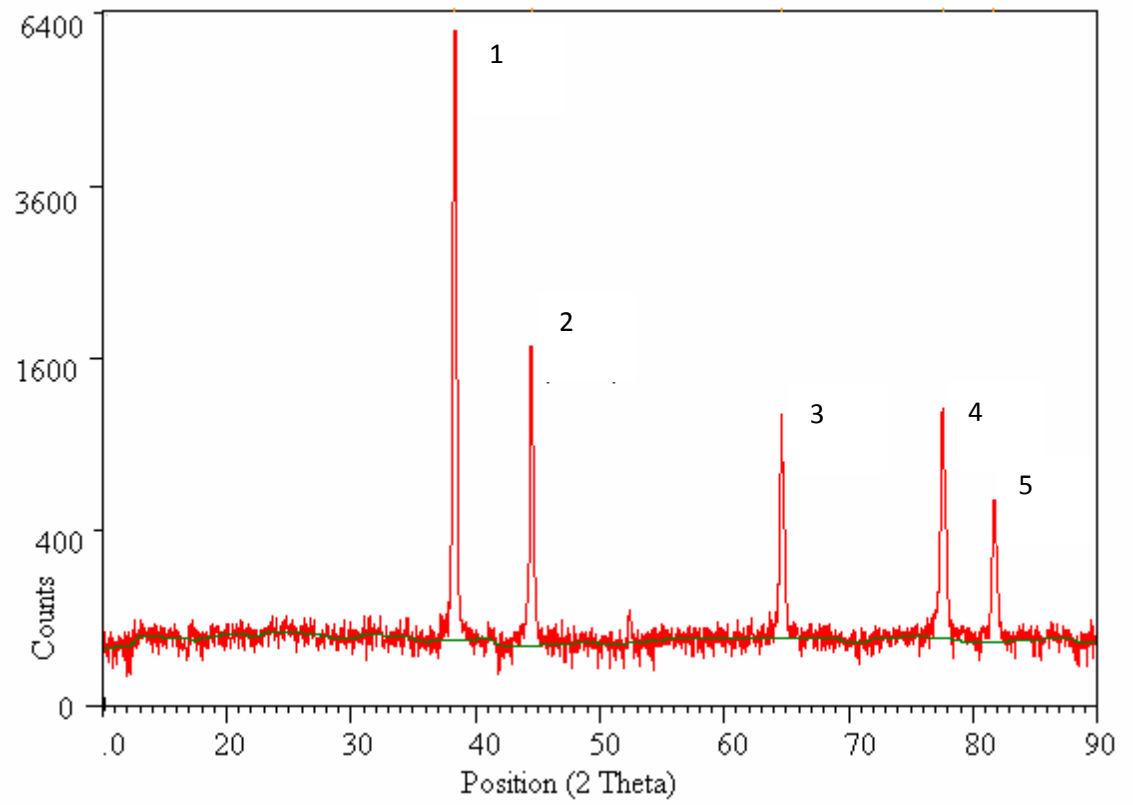

Fig. 1. ***The*** **X-ray diffraction pattern of the silver nanoparticles** ***showing the Peak lines and 2θ Positions***

(Cornell University Library **, arXiv:1111.0260)**