**[MS26-P04] Microstructural investigation: *Xbroad* – computer program for XRD size-strain analysis**

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Understanding the defect structure of the material has become a priority objective in research targeted on the development of new materials since crystallite size, crystallite size distribution, microstrain, dislocation density and stacking fault probability play a major role in the final properties of the material. Since preparation of new nanomaterials with controlled particle size and shape became essential for tailoring the desired material properties, a quick and effective XRD line broadening analysis became an imperative. Although the methods implemented in the program are considered to be *traditional* ones, the authors believe that the program provides a very fast platform for non-crystallographers working in the field of materials science. The first step in the X-ray broadening analysis performed by XBroad is a correction for instrumental broadening which is done by the rigid Stokes deconvolution. The Stokes deconvolution has so far remained the only totally unbiased method since no assumptions on the line profile shapes are made. A valuable characteristic of the Stokes method is that any degree of broadening of the diffraction profile due to the angular separation of the $K\_$ doublet is automatically allowed for. After correction for instrumental broadening, the program performs analysis based on two methods: (i)Warren-Averbach-Bertaut (WAB), (ii) Williamson-Hall (WH). In the WAB method, the Fourier coefficients F(L) of the pure diffraction profile (obtained in the first step) are plotted versus their order L. The program calculates the average area-weighted column length from from the inverse slope of F(L) when L approaches zero. In the WH analysis, the calculated breadth of the pure diffraction profile, _i, is used to calculate average volume-weighted column length and the upper limit of lattice strain. Program and tutorial can be downloaded from:

http://www.phy.pmf.unizg.hr/~zskoko/Fizika_mat_web/XRD.html

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