THE DIRECT DETERMINATION OF X-RAY DIFFRACTION DATA FROM SPECIFIC DEPTHS

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The ability to characterise polycrystalline thin films with depth is of great interest in materials science, as knowledge of structural characteristics aids in the understanding of thin film behaviour and optimises manufacturing processes. Many current approaches to depth profiling are destructive, i.e. a small amount of material is systematically removed from the uppermost layers, either by polishing or cutting.

In order to analyse samples in a non-destructive manner, the effective depth of analysis may be reduced by reducing the angle between the incident analysing probe and the sample surface. For any given incident angle, the diffraction data obtained is an average of information from various depths over the depth of penetration, weighted towards the uppermost layers. Until now, information from a specific depth below the surface of the sample could not be directly determined from this observed diffraction data. By transforming experimental angle-dependent data, we have introduced a method of directly determining diffraction data arising from specific depths beneath the surface. This can then be exploited using any conventional method, e.g. Rietveld analysis.

Previous works by a variety of groups have produced depth-profiles on the scale of absorption depth. Our method includes changes in the linear absorption coefficient with depth. In addition, discontinuities have previously not been accommodated into algorithms for determining depth profiles, whereas in our work, this can be accommodated.

We will present the method used and its validation by the generation of pseudo-experimental data and the recovery of the depth-dependent solution. The application of the algorithm to experimental data from a number of polycrystalline thin film systems, collected using asymmetric parallel beam geometry, will also be presented.