

A New Approach to High Throughput Diffraction Analysis

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Thin film, continuous compositional spread (CCS) libraries are made by creating a gradient across a substrate using two or more chemical compounds. Conventionally analytical probes are used in a raster scanning mode to characterize the libraries. We have been exploring methods of significantly reducing the characterization time using an X-Ray ‘line’ probe to simultaneously illuminate multiple points on the library and an area detector to collect the superposed scattering data. This data is then transformed (‘partitioned’) using new software, ‘Bandit’ into scattering data arising from each source along the line probe. Thus diffraction data from all points along one dimension of the library is accessible and produced at a fraction of the time of a conventional raster scan. Bandit applies an external standard calibration to ensure accurate d-spacing determinations from each intensity maxima. The mathematical transformation is then applied to produce the corresponding intensity, d-space and position on the samples contour plots. We will present this data and contrast it with that from conventional raster scans from the same libraries. We show that the algorithm provides reliable data and a significant increase in the interrogation speed of X-ray diffraction.

CuSb binary libraries were electrodeposited on molybdenum coated glass substrates. Contour plots corresponding to the CuSb libraries are shown in **Error! Reference source not found.** Cu and Mo peaks are the only ones visible at 16 mm. At 18 mm the peaks have been assigned to Cu, Mo and Cu₁₁Sb₃. Mo, Cu₂Sb and Cu_{3.3}Sb co-exist at 20 mm while Cu₂Sb and Sb are the only alloys detected from 26mm to 31 mm together with the signal coming from the substrate. From 33 mm only elemental Sb can be detected. From these graphs is possible to observe how the number of peaks and their positions match for the two methods.

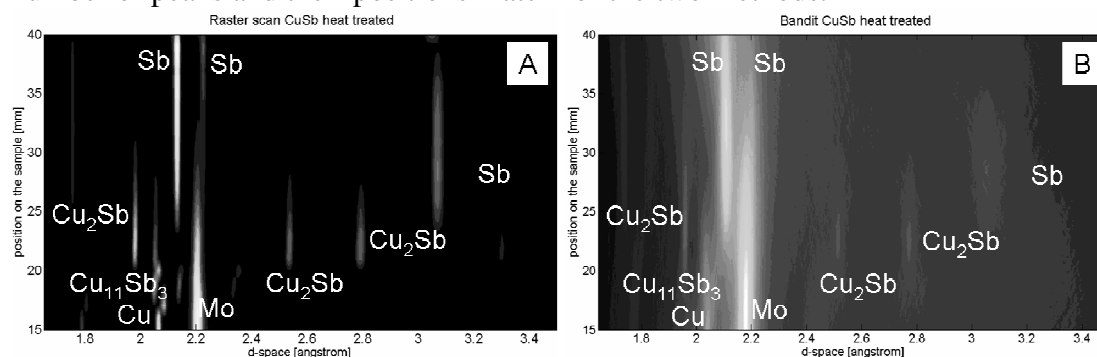


Figure 1: Contour plots of CuSb libraries for raster scan (a) and Bandit (b) methods