Spiral Powder Overlays

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Spiral overlays, for use with powder diffraction patterns and diffraction spacing profiles, can be at once forgiving of uncertainties in camera constant calibration and (once these are dealt with) sensitive to very small differences in lattice parameter. By facilitating comparison of different lattices in a common physical metric (namely a diffraction experiment of fixed camera constant and scattering center density), their pedagogical value also extends to the comparison of crystal structures whose atomic environments share physical features (like nearest neighbor distances) in spite of major differences in symmetry. The overlays can be put onto transparencies for use directly with negatives and hardcopy, or in digital form for use with digitized images [1].

Figure 1 illustrates analysis of the experimental electron diffraction pattern from an unknown assemblage of nanocrystals (red), against overlays (green) for body-centered, face-centered, and diamond cubic lattices. In blue find notations concerning the line of spacing matchups, as well as where various elemental compounds would plot if one had calibrated the camera constant of the pattern precisely. (This was not the case for this analysis.)

Fig. 2 shows a comparison of face centered cubic (f.c.c.) and hexagonal close packed (h.c.p.) overlays, illustrating what the associated lattices do and do not have in common. *Tip: To see the fcc or hcp overlays alone, look through a pair of red-green glasses with but one eye open, so that you see only red (fcc) or green (hcp).* Why do the diffraction spacings show so much overlap (yellow)? An atom-thick hexagonal array of atoms can be naturally stacked against a second array in one of only two ways, if the distance between nearest atoms is to be the same within and between arrays. Denote the alignment of the first array with the letter "A". The two possible adjacent layers then have "B" and "C" alignments. If one stacks such layers in the sequence ABCABC, one gets a face-centered cubic lattice (which strangely enough has four equivalent "stacking directions" along body diagonals of the cubic unit cell). Restacking of them in ABABAB form instead yields the corresponding hexagonal close-packed structure, which is not similarly isotropic (hence more spacings created than lost). In fact all f.c.c. spacings graphed are h.c.p. spacings too, except those of the form (h00).

Fig. 3 shows an f.c.c analysis of the experimental 300kV electron diffraction pattern from a polycrystalline Al thin film. In spite of the overlay's ability to reveal spacing matches even if the lattice parameter (or the camera constant of the pattern) is completely unknown, note how easily the angle of the match line for a carefully calibrated pattern allows us to distinguish between very similar lattices of Al and Ag.

References

[1] Resources for doing this will be linked to http://www.umsl.edu/~fraundor/pdifovly.html

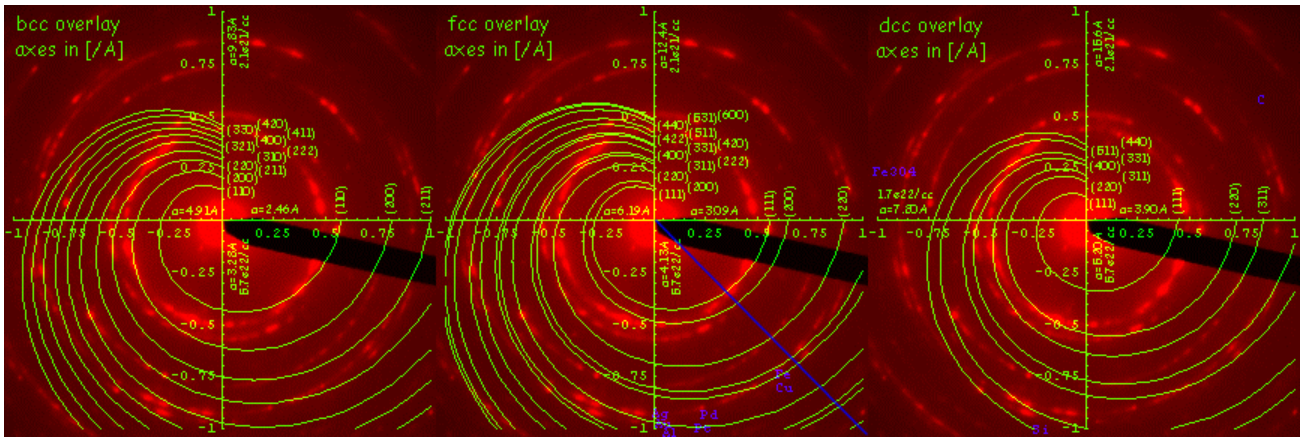

FIG. 1. Spiral body-centered, face-centered, and diamond-centered cubic overlays (green), used to identify a pattern of unknown camera constant (red) as face centered cubic (blue line).

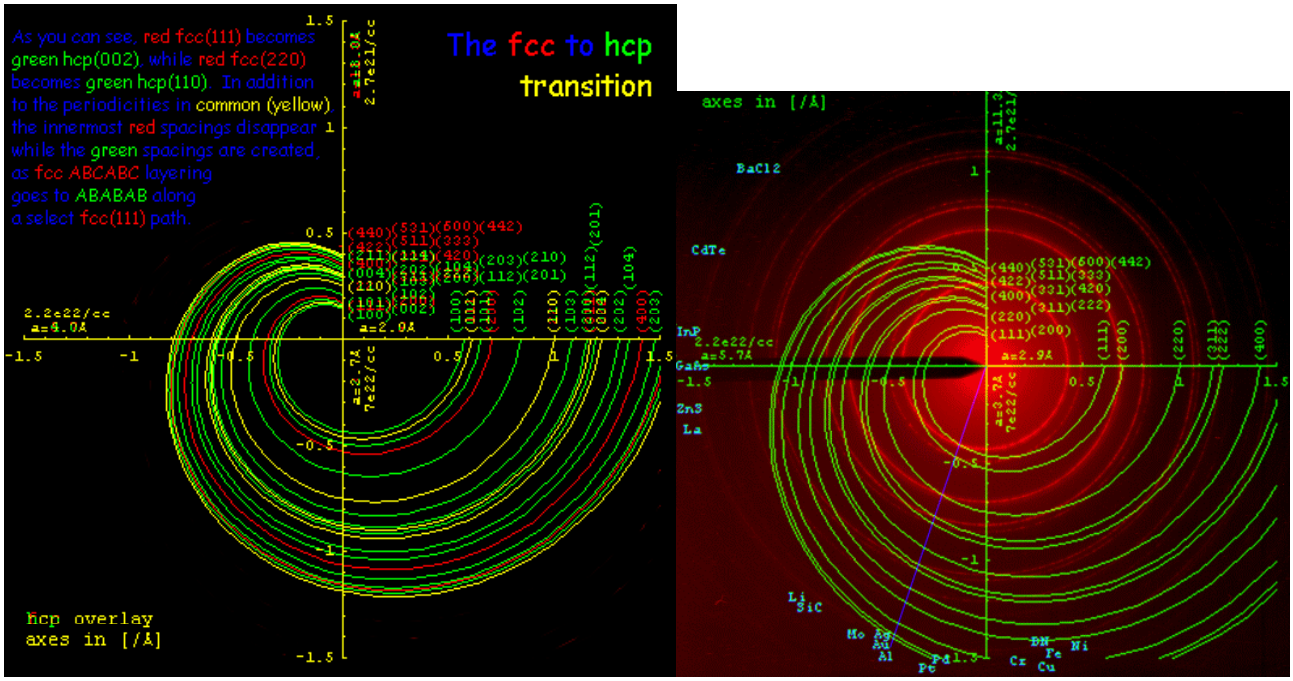

FIG. 2. (left) Spiral overlays for face-centered cubic and hexagonal close-packed crystals with identical interatom spacing, illustrating what changes and what stays the same as the crystal re-orders from ABCABC to ABABAB layering along one of the cubic three-fold symmetry axes.

FIG. 3. (right) Face-centered cubic overlay (green) used to distinguish Al from Ag (blue line) as the source of a pattern of well known camera constant (red).