On-line determination of nanocrystal lattice parameters

*Question:* Is near-automatic on-line measurement of Bravais lattice parameters for an arbitrary nano-crystal possible with a sub-Å microscope? *Answer:* Yes, IF…

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EMS OnLine for Model Drawings
(http://cimewww.epfl.ch/CIOL/)
1. Mirror symmetry about lattice planes
2. Azimuthal symmetry of e-beam about lattice plane normal (spherical crystal)

Each point in the band: An e-beam direction in which the fringe is visible.
Sample Visibility Band Map

Uses include:

- “Kikuchi Map” in direct space, useful as roadmap to guide crystallographic analysis. Band width \( d \) & \( 1/(\text{crystal thickness}) \)
- Calculating fringe probabilities with random orientation, and fringe correlation “fingerprints”
- Calculating projection errors in fringe spacing

What happens as the contrast transfer function improves?
Below: visibility bands for 80Å Al-crystal @ 1Å resolution
At 0.6Å resolution, of course fringes may be seen at most orientations. Now, what if the grain size is even smaller?

For 30Å grains, the visibility bands have widened, so seeing fringes tells us less about orientation. What now?
Given fine 2D tilt control, an elegant protocol follows…

* Find “large” spacing.
* Maximize it.
* Tilt along it to 1st cross fringe set A.
* Maximize cross fringe.
* Tilt along it to 2nd cross fringe set B.
* Etc. to C, D, over full tilt range…

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Discussion/Summary

- Three non-coplanar spacings yields a subset of, & often the full, 3D reciprocal lattice.
- N spacings from N-1 zones over the available tilt range yields/minimizes errors as described in *Ultramicroscopy* 6 (1981) 227-236.
- TEAM design request: develop fine (e.g. 0.1 degree) automated double-axis tilt control.