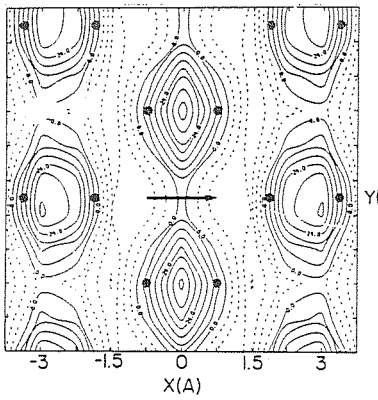
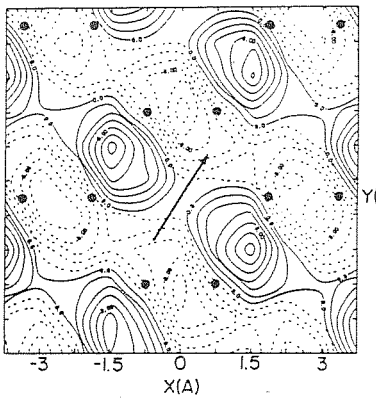
14.4-14 OBTAINING ATOMIC COORDINATES FROM ELECTRON MICRODIFFRACTION PATTERNS by John Konnert and Peter D'Antonio, Laboratory for the Structure of Matter, U.S. Naval Research Laboratory, Washington, D.C.

Diffraction data has been obtained from regions as small as 3A in diameter using an HB5 STEM from VG Microscopes, Ltd., that has been fitted with a special ultra-high resolution pole-piece (Cowley, Ultramicroscopy, 1984, 14, 27-36). An image reconstruction procedure has been described (Konnert and D'Antonio, Ultramicroscopy, 1986, 19, 267-277) that utilizes microdiffraction patterns from overlapping regions of sample. The Fourier transforms of the intensities or autocorrelation functions (ACF) are calculated for an array of beam positions surrounding the sample area of interest, and the beam positions that maximize each ACF vector are identified. Because such maxima occur with the beam nearly centered between related atoms, each resolved maximum serves to identify the positions of two atoms. The microdiffraction patterns do not in general possess a center of symmetry. Thus their Fourier transforms are complex. The real part of the ACF is the real part of the electron wave function at the exit surface of the sample convoluted with itself plus the imaginary part convoluted with itself. A peak in the real part of the ACF is more likely to arise from two atoms in the central portion of the beam than is a peak in either the full ACF or its imaginary part. The accompanying figures derive from theoretical diffraction data calculated for 100A thick Si viewed along [110]. They display the variation with beam position of the real part of the ACF for two vectors. Each maximum determines two atom positions. A corresponding display for the ACF origin (annular detector data) possesses maxima midway between the closer pairs of atoms. Quite accurate diffraction data is required to obtain the required information on non-zero ACF peaks. Experiments are being carried out at Arizona State to evaluate the usefulness of the procedure.



Real part of the autocorrelation function vs. beam position for the (x=1.36A, y=0A) vector. The dots represent columns of atoms. Note that the maxima occur with the beam centered between atoms related by the ACF vector. Beam stepped in increments of 0.75A.



Real part of the autocorrelation function vs. beam position for the (x=1.36A, y=1.36A) vector. Maxima occur with the beam centered between atoms related by the associated vector.

14.4-15 BOUNDARY STRUCTURE ANALYSIS OF LAYERED LATTICE - MODIFICATION OF CSL MODEL. By Y. Kitano, M. Takata and Y. Komura, Department of Materials Science, Hiroshima University, Japan.

Coinsidence Site Lattice (CSL) model is modified in order to interpret boundary structures of crystal interfaces of layer structures such as Mg-base Laves phase alloys. Since identical layers stack on top of each other in a layer structure, all the origins in each layer can be adopted as lattice points for drawing interpenetrating lattices. Interpenetrating lattices exhibit some clusters of coincidence sites and produce a characteristic pattern with an appropriate period. This pattern is one of main results of a modified CSL (M-CSL) model and is called an M-CSL-Pattern. An example is shown in Figure below for 2H/9R boundary. An M-CSL-Pattern is directly observed in high resolution micrographs (HREM) of twist boundary. The M-CSL model has been employed to analyse 70.5° tilt boundaries of

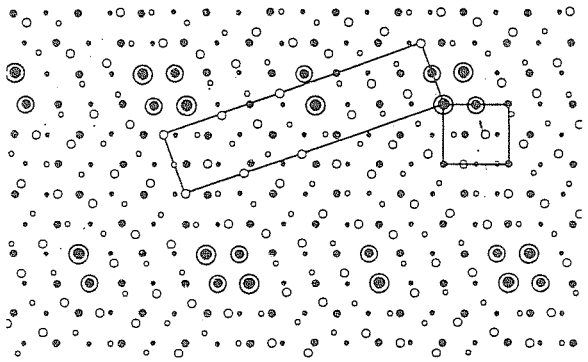


Figure: M-CSL-Pattern of 70.5° boundary of 2H/9R. Double circles indicate coincidence sites.

2H/2H, 4H/4H and 2H/9R for the Laves phase alloys by Takata, Kitano and Komura (1985 Abs. autumn Meeting JIM 447; 1986a Trans. JIM **27** Supplement 261; 1986b Abs. spring Meeting JIM 260) and that of 6H/6H for SiC by Ichinose and Ishida (private communication).

Σ is defined in interpenetrating lattices as a reciprocal ratio of a number of coincidence sites to all the lattice points. Σ_0 (Σ based on a CSL model) must be modified by multiplying a factor R, because extra coincidence occurs in the M-CSL model. If $R < 1$ and a new Σ ($\Sigma_0 \times R$) $< \Sigma_0$, then a ratio of coincidence sites to all the lattice points increases. Σ_0, R, $\Sigma_0 \times R$ are listed in Table below for several interfaces.

An boundary dislocation with a step or a stacking fault observed in an HREM image is characterized by DSC lattice vectors based on M-CSL model (Takata et al. 1985, 1986a, 1986b). Shifting one of two adjacent crystals by a DSC lattice vector, M-CSL-Pattern should be reproduced. This statement is true for most cases of layer stuctures but for a few cases such as a 70.5° boundary of 6H/6H, where several times of shift by a DSC lattice vector are required for reproduction of M-CSL-Pattern. Here a large R factor 3 or 4 in Table corresponds to an intermediate state. Therefore a boundary dislocation of 6H/6H would have a larger Burgers vector.

Since M-CSL-Pattern has a close relation to coincidence atomic sites in a rather complex crystal structure, M-CSL-Pattern directly gives details of atomic configuration at a boundary.

Boundary	Σ_0	R	$\Sigma_0 \times R$
2H/2H	9	1	9
4H/4H	18	1/2	9
6H/6H	3	3/4, 3, 4	9/4, 9, 12

Table