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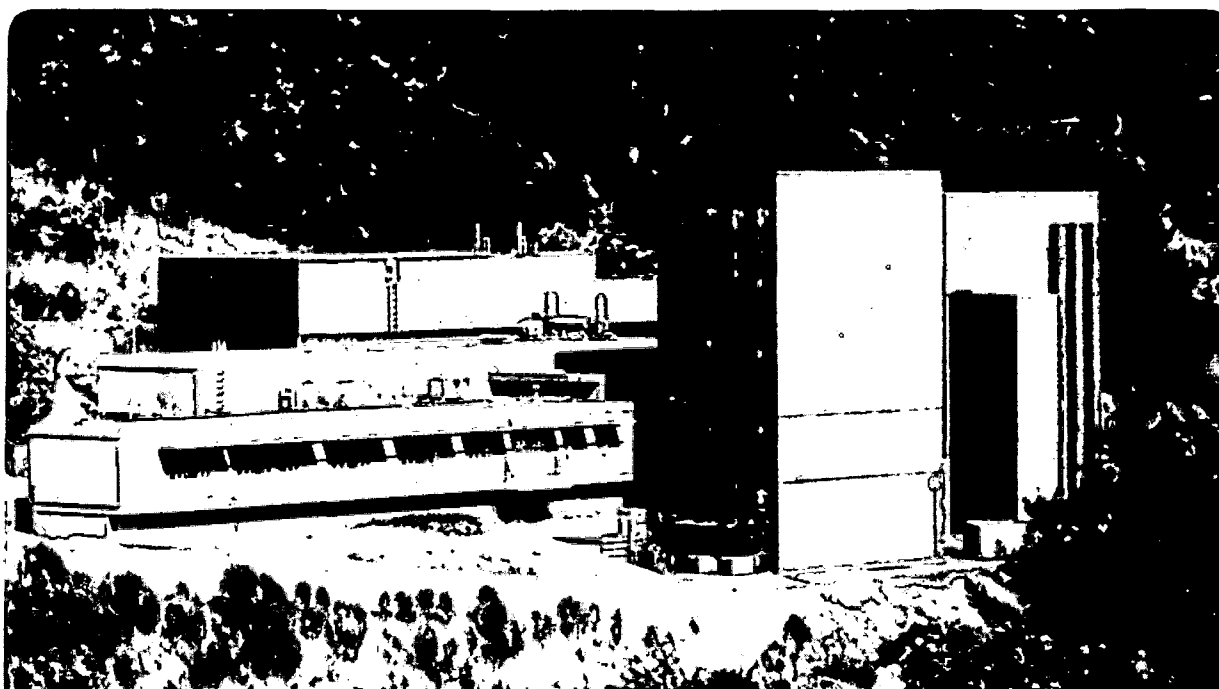
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SIMULATED IMAGE MAPS FOR USE IN
EXPERIMENTAL HIGH-RESOLUTION ELECTRON MICROSCOPY

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SIMULATED IMAGE MAPS FOR USE IN EXPERIMENTAL HIGH-RESOLUTION ELECTRON MICROSCOPY

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ABSTRACT

A "map" of all possible high-resolution images may be simulated for a crystalline specimen in a chosen orientation for any particular transmission electron microscope (HRTEM). These maps are useful during experimental high-resolution electron microscopy and make it possible to locate optimum imaging conditions even for foil thicknesses beyond the weak-phase object limit. Although defects such as grain boundaries are not generally periodic, image maps of perfect crystal can be used to optimize defect contrast during operation of the microscope by reference to the image of the perfect crystal neighboring the defect.

INTRODUCTION

The current availability, at reasonable cost, of high-speed computing has made feasible the rapid generation of simulated images. A useful application [1] of these advances is the production, before the experiment, of all possible images (rather than a select few after the event). For perfect periodic crystals, image contrast conditions repeat with both crystal thickness and microscope defocus, allowing a map to be made that includes all possible HRTEM images. Inclusion of partial coherence limits the map to the range of defocus that can be used experimentally. For a crystal with repeat distance \mathbf{d} of 2 to 3 Ångstrom units (in projection), the Fourier image defocus period $2\mathbf{d}^2/\lambda$ is small enough to allow a useful map to be produced as an array of about ten to fifteen defocus values by ten to twenty thickness values; typical steps might be 100Å in defocus and 20Å in thickness.

THEORY

The ranges of values of microscope defocus and specimen thickness over which an image map should extend may be determined by consideration of Fourier-images and dynamic extinction distance. Fourier-image theory [2] has been shown to be useful in experimental measurement of defocus values in high-resolution electron microscopy [3], and the concept of Fourier-image defocus period provides a means of defining the focus range over which changes in defocus can produce new image contrast. The phenomenon of near-repetition of image contrast with increasing crystal thickness is due to the effect of dynamic extinction distance [4], and depends upon both specimen structure and orientation, as well as the electron wavelength used.

The overall phase of a diffracted beam may be written as

$$\phi(\mathbf{k}) = \pi/2 + \phi_{\text{dyn}}(\mathbf{k}) + \chi(\mathbf{k}) \quad (1)$$

where $\pi/2$ is the phase change on kinematic scattering, $\phi_{\text{dyn}}(\mathbf{k})$ is the additional change due to dynamical effects, and $\chi(\mathbf{k})$ is the phase change imposed by the objective lens [3]. The dynamical term, $\phi_{\text{dyn}}(\mathbf{k})$, varies with crystal thickness, and, for simple metals and semiconductors is near-periodic with the period of the dynamic extinction distance if absorption is neglected [4]. Therefore, for a given lens defocus, and for HRTEM specimens thin enough for absorption to be negligible, $\phi(\mathbf{k})$ can be periodic in crystal thickness to quite a good approximation. Similarly, for any given specimen thickness, the lens term, $\chi(\mathbf{k})$, [and hence $\phi(\mathbf{k})$], is periodic with objective lens defocus with a period of $2\mathbf{d}^2/\lambda$, where \mathbf{d} is the (projected) unit cell length [2].

EXPERIMENTAL

To determine optimum viewing conditions for an interface in aluminum, (in this case a $\Sigma 99$ {557} $\langle 110 \rangle$ tilt boundary), we considered images of perfect aluminum up to 440Å thick, over one Fourier-image period of $2d^2/\lambda$ for experimental conditions corresponding to the NCEM Atomic-Resolution Microscope (JEOL ARM-1000).

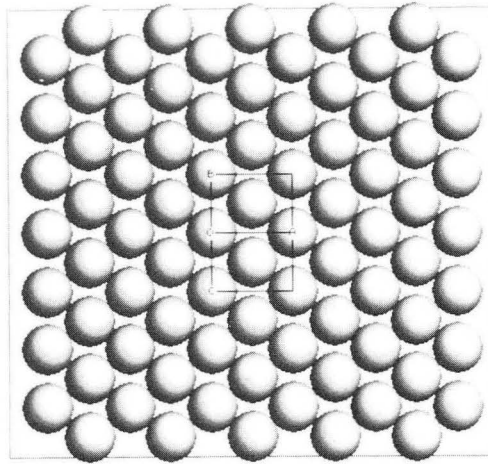
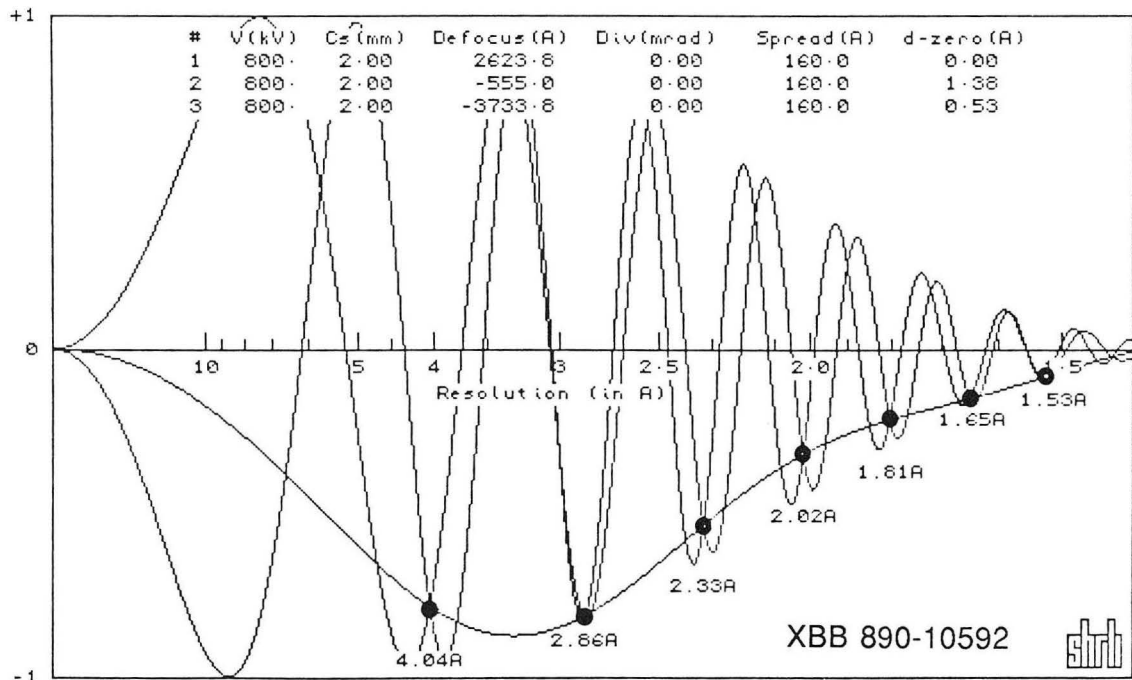


Figure 1. Model of aluminum in [110] projection showing the original cell and the cell of size $|a|$ by $|a|/\sqrt{2}$.

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In [110] projection, the smallest orthogonal cell in perfect aluminum (fig.1) is $|a|$ by $|a|/\sqrt{2}$, or 4.04Å by 2.86Å. These dimensions yield Fourier-image periods of 3178Å and 1589Å respectively for an electron wavelength corresponding to the experimental energy of 800keV; the overall period is the lowest common multiple, or 3178Å. A plot of contrast-transfer functions (CTFs) at three values of defocus differing by 3178Å confirms that $\chi(k)$ values for all three are identical at spatial frequencies equal to $\sqrt{n}/|a|$ (fig.2).



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Figure 2. CTFs for defocus values separated by one Fourier image period for ARM conditions (listed at top) and $|a| = 4.04\text{Å}$. Positions where all three curves intersect are marked and labelled with real-space distances equal to $|a|/\sqrt{n}$ for $n=1$ to 7.

RESULTS

Images simulated using the NCEMSS programs [5] over the defocus range $+381\text{\AA}$ to -3175\AA show a defocus period of 3175\AA , corresponding to the Fourier-image value. Four types of high-contrast images occur (fig.3). At Scherzer defocus (-500\AA), thin-crystal images have black spots at atom positions (S-type images). Near -900\AA defocus, white spots appear at atom positions (W images). Images near defocus values of -1500\AA and -2500\AA are white-spot images like that near -900\AA , but shifted by a half unit cell (\bar{W} images). Similarly, the image at -2000\AA defocus is a black-spot image displaced by a half cell (\bar{S} image). Images at 0\AA and -3175\AA (a Fourier pair) are W images.

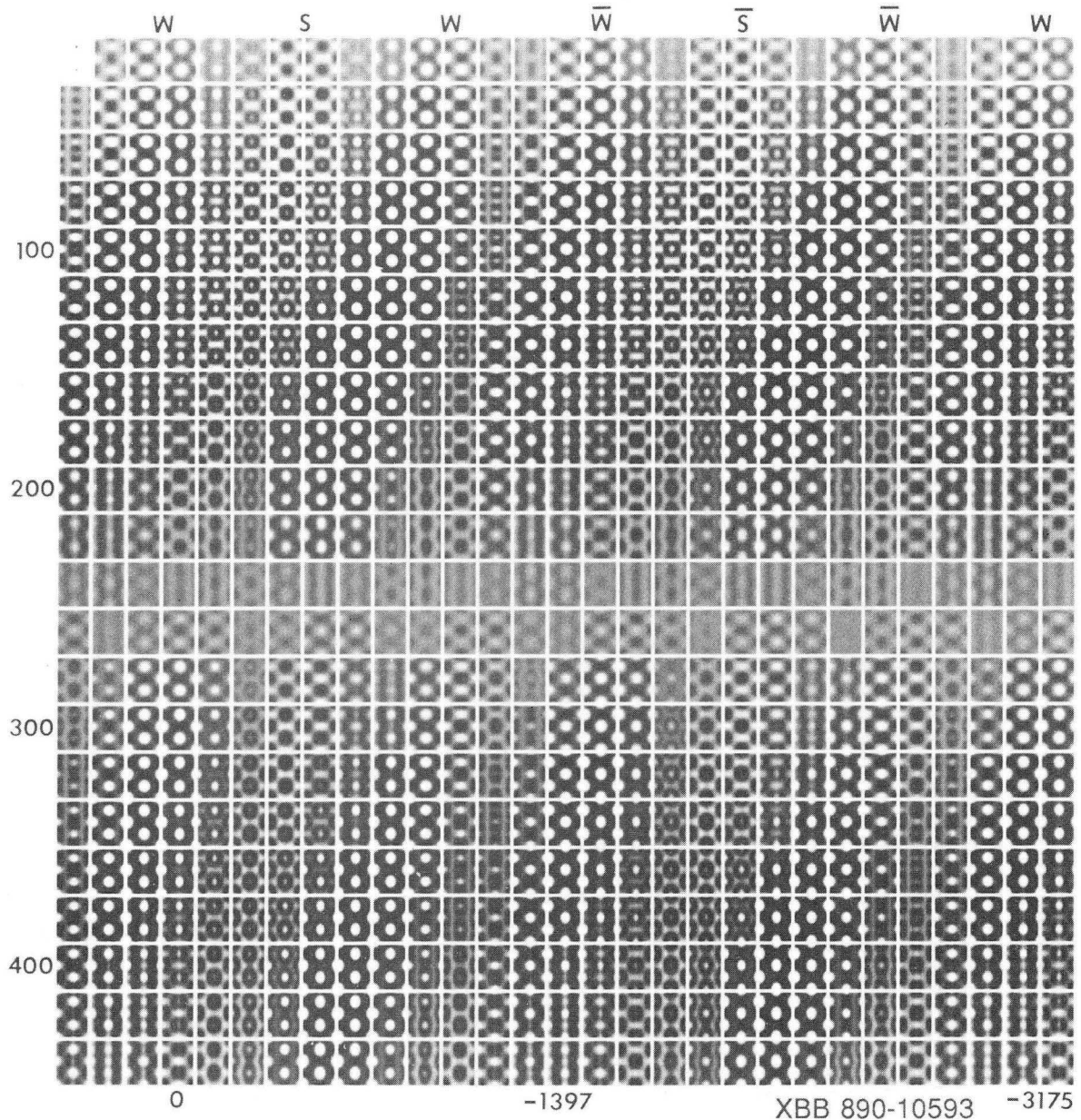


Figure 3. Images simulated for ARM conditions covering the defocus range horizontally from $+381\text{\AA}$ to -3175\AA in 29 steps of 127\AA and the crystal thickness range vertically from 20\AA to 440\AA in 22 steps of 20\AA . Display contrast is held identical for all images, allowing the loss of contrast at the extinction thickness of 240\AA to be seen clearly. For comparison with the images, the positions of atoms within the cell are displayed as black dots in the projected potential plot (top left).

Figures 2 and 3 were computed without the effect of incident electron beam convergence (spatial coherency) in order to demonstrate the periodicity of images with defocus. When convergence is included at the level corresponding to the condenser aperture commonly used in the ARM, it is found that the range of useful images is less than one complete Fourier-image period. The beam-dampening effect of convergence is weak near Scherzer defocus, but stronger as defocus is increased or decreased [6], resulting in very low contrast far from Scherzer defocus (fig.4). These lower-contrast images are not experimentally useful and may be neglected, condensing the required image map to a defocus range of approximately one half of the Fourier-image period.

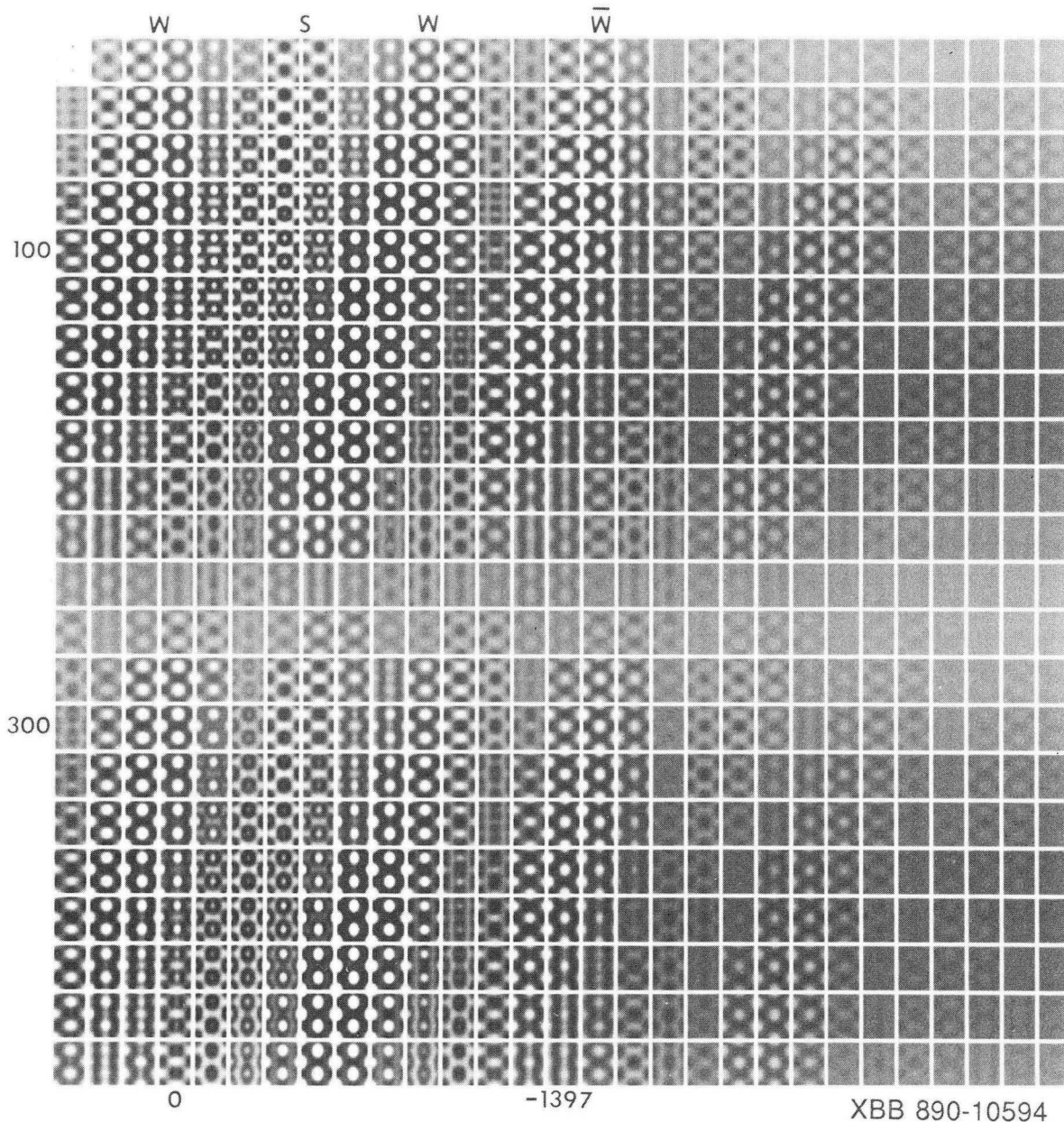


Figure 4. Images computed for the conditions of figure 3, but including an incident beam convergence of 0.6 millirad. halfangle, corresponding to the measured experimental value. As defocus becomes larger, images lose resolution, then contrast.

Because underfocus conditions generally result in higher resolutions [7], a useful image map for [110] aluminum imaged in the ARM at 800keV need cover only the range from zero to approximately -1400\AA . This map (fig.5) clearly shows the 260\AA repeat in thickness, and the high-contrast regions that become skewed in the direction of positive defocus as crystal thickness is increased [8]. From the image map (fig.5), the white-spot (W) images near -800\AA defocus and 100\AA thickness show good fidelity (each white spot is centered on an atom position) and possess higher contrast than the black-spot (S) images near Scherzer defocus (-500\AA). For these reasons, the "best" conditions of -800\AA defocus and 100\AA thickness were selected when an experimental image of a $\Sigma 99$ $\{557\}$ $\langle 110 \rangle$ tilt boundary in aluminum was obtained. Figure 6 shows a comparison of the experimental image with one simulated from a grain-boundary model [9].

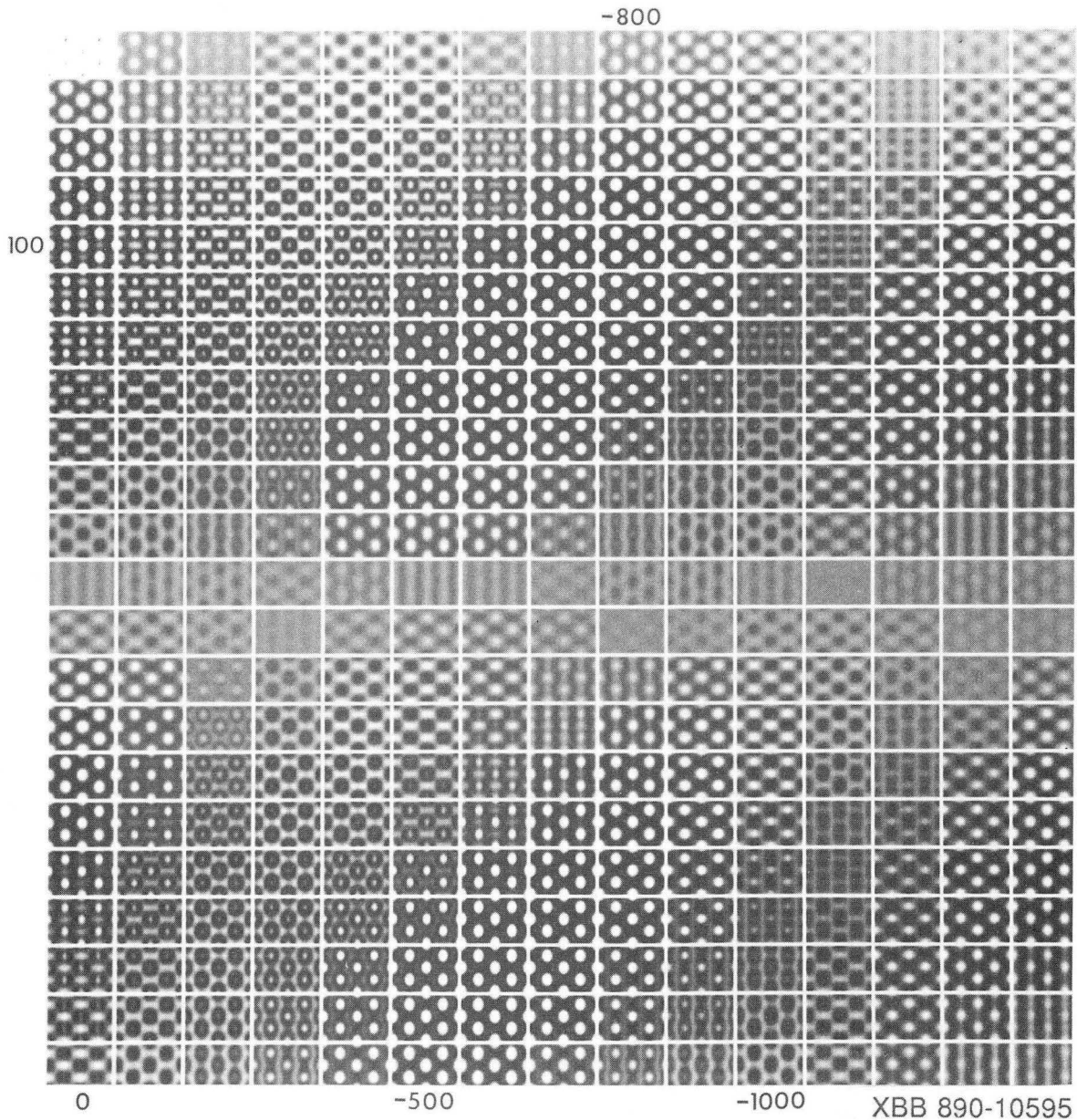
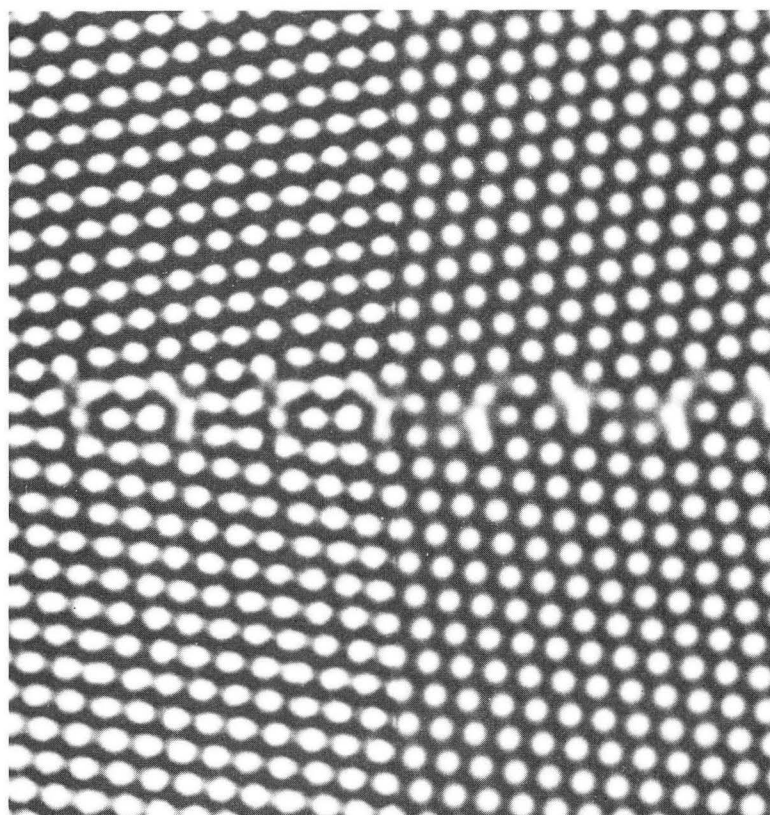


Figure 5. Final image map for [110] aluminum under ARM conditions. Defocus values (horizontal) are from 0 to -1400\AA in steps of -100\AA . Thickness values (vertical) are from 20\AA to 440\AA in steps of 20\AA . Atom positions (black dots) are shown top left.



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Figure 6. Comparison of experimental image (left) of $\Sigma 99$ {557} $\langle 110 \rangle$ tilt boundary in aluminum with image (right) simulated at a defocus value of -800\AA and 103\AA crystal thickness. The simulation conditions correspond to those of the JEOL ARM-1000 operated at 800keV : $C_S = 2.0\text{mm}$; spread of focus = 160\AA ; beam convergence = 0.6millirad . A Gaussian vibration corresponding to 0.5\AA halfwidth at the specimen is included.

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