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To be presented at the 46th Annual Meeting of the Electron Microscopy Society of America, Milwaukee, WI, August 7–12, 1988

Identification of Periodic Structure Characterized from Amorphous Support by Simulation and Processing Techniques

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April 1988

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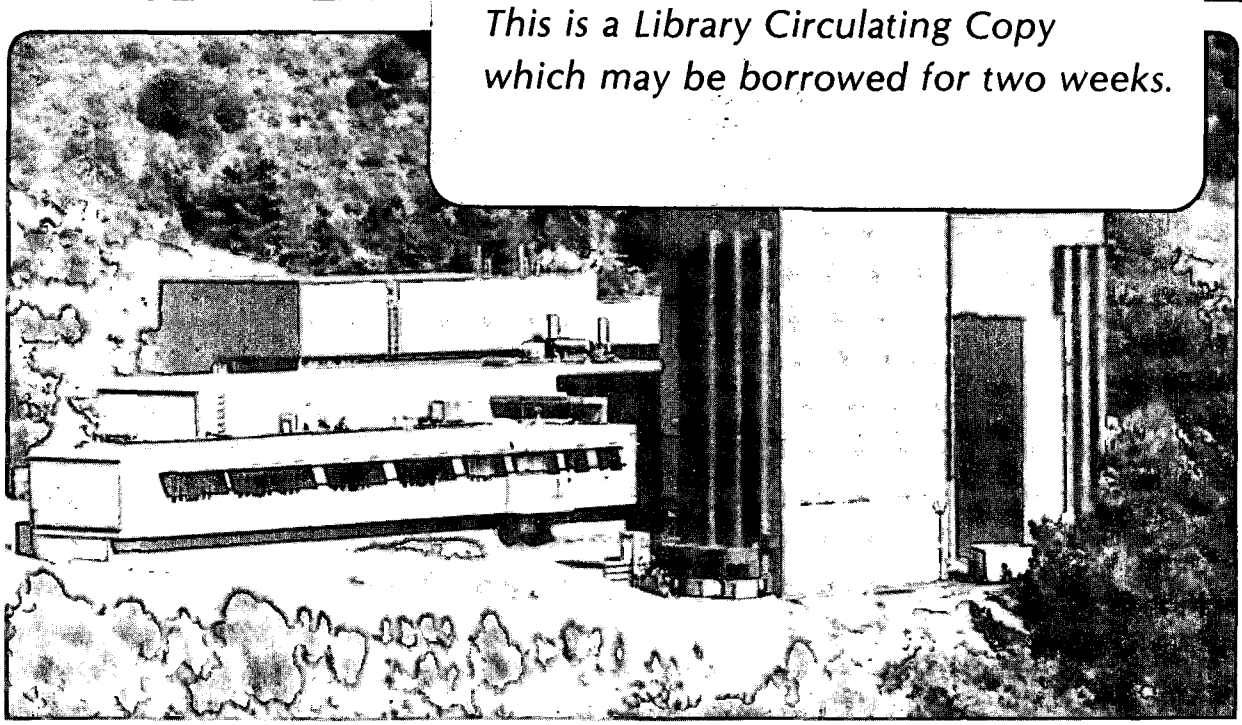

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Prepared for the U.S. Department of Energy under Contract Number DE-AC03-76SF00098.

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IDENTIFICATION OF PERIODIC STRUCTURE CHARACTERIZED FROM AMORPHOUS SUPPORT BY SIMULATION AND PROCESSING TECHNIQUES

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High resolution electron images that suggest crystalline lattice fringes in a background of amorphous material are difficult to interpret. A new technique of image processing, referred to here as "background subtraction", was recently developed[1] to enhance images of such crystalline particles supported on amorphous substrates. However, the interpretation of exact crystalline surfaces on the particle was not straightforward. We have now applied this enhancement technique, previously used on experimental images, to simulated images of small crystals on amorphous substrates. Additionally, other commonly-used processing techniques are introduced as comparisons for the "background subtraction" method to point out its advantage in defining particle shape and internal structure.

The model used for simulation consists of eight by eight units of anatase in [111] orientation (Fig. 1), enclosed in a "unit cell" of 56.8Å by 56.8Å (corresponding in size to 16 by 16 units of anatase). In addition we added various thicknesses of a structure of random SiO_2 units to this model to simulate the effects of an amorphous support. The SHRLI programs[2] were used to generate images from this model for 11Å of anatase supported on 0Å, 11Å, 33Å, and 55Å of amorphous substrate (Fig. 2) for experimental conditions suitable for the atomic resolution microscope at the NCEM (800keV and C_s=2.36mm with an objective aperture of 0.55 reciprocal Å, an incident beam convergence semiangle of 0.6 milliradian, and a spread of focus of 100Å).

The background-subtraction enhancement technique separates the amorphous support contribution to the image intensity spectrum from that due to the crystalline particle by first setting Bragg spots in the Fourier transform to the local mean intensity. A back transform is then applied to obtain the aperiodic part of the total image, and this is subtracted from the original image to leave only the periodic part due to the crystalline particle. This method is designed to preserve the shape transform of the particle in diffraction space. Figure 3 gives results from applying this technique to images of the crystalline anatase particle supported by varying thicknesses of amorphous silica. Examination of the last two images reveals that the background-subtraction method fails to reproduce the particle shape when the amorphous:crystalline thickness ratio exceeds approximately 4:1 or 5:1.

Results of the background subtraction technique were compared with results from other conventional enhancement methods. Figure 4 shows these results for a simulated image at 4:1 amorphous to crystalline thickness ratio. Of all the methods shown, the Gaussian annular ring technique[3] preserves the particle shape best, but includes information from the amorphous background, giving the extracted particle image an internal structure similar to the original image; this technique also leaves random spots present ouside the crystal, in the surrounding amorphous image. The commonly used window method for processing bulk crystalline images overestimates particle shape with periodic fringes that "ring" out from the particle surfaces. Of all the methods tested, the background subtraction method seems to preserve particle shape best with the least amount of ringing and no amorphous contribution to the extracted particle image.

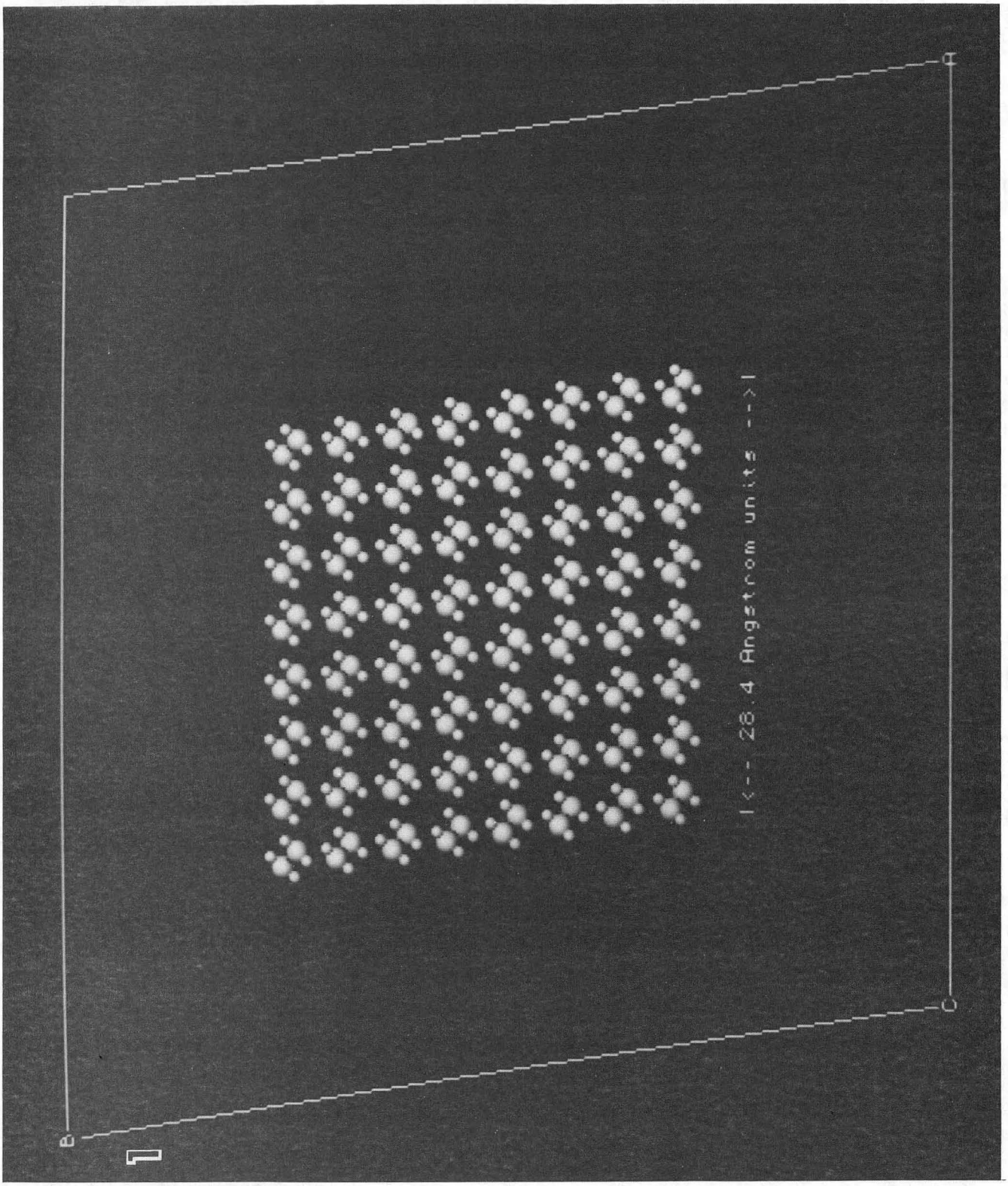
1. M. L. Sattler and M. A. O'Keefe, Proc. 45th EMSA (1987)104-105.
2. M. A. O'Keefe and P. R. Buseck, Trans. ACA 15 (1979) 27-46.
3. W. O. Saxton, Proc. 44th EMSA (1986) 526-527.
4. This work is supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Science Division, U.S. Department of Energy under Contract No. DE-AC03-76S F00098.

Figure 1. Model of anatase (TiO_2) crystal of size 8 by 8 units viewed along [111]. Large spheres represent Ti atoms, smaller ones 0 atoms.

Figure 2. Simulated images of model crystal 11Å thick supported on 0Å, 11Å, 33Å, and 55Å of amorphous SiO_2. Ratio indicates amorphous to crystalline thicknesses.

Figure 3. Processed images of crystal plus support, using background subtraction technique o the images above.

Figure 4. Comparison of results from four different processing techniques using 4:1 model.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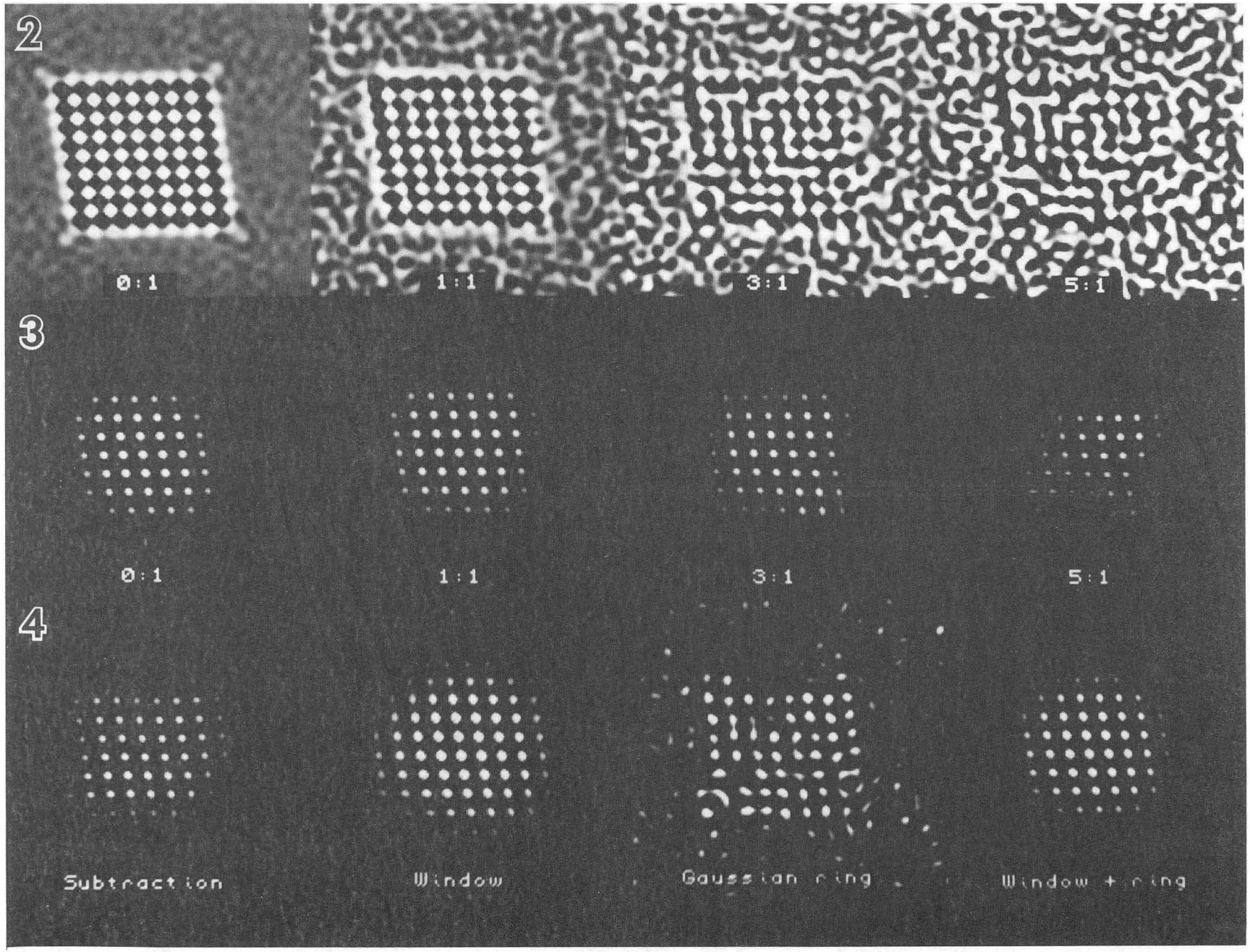
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3
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5:1
4
Subtraction
Window
Gaussian ring
Window + ring

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