LBL-30690

Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

Materials & Chemical Sciences Division

National Center for Electron Microscopy

Presented at the Electron Microscopy Society of America/Microbeam Analysis Society Meeting, San Jose, CA, August 4–9, 1991, and to be published in the Proceedings

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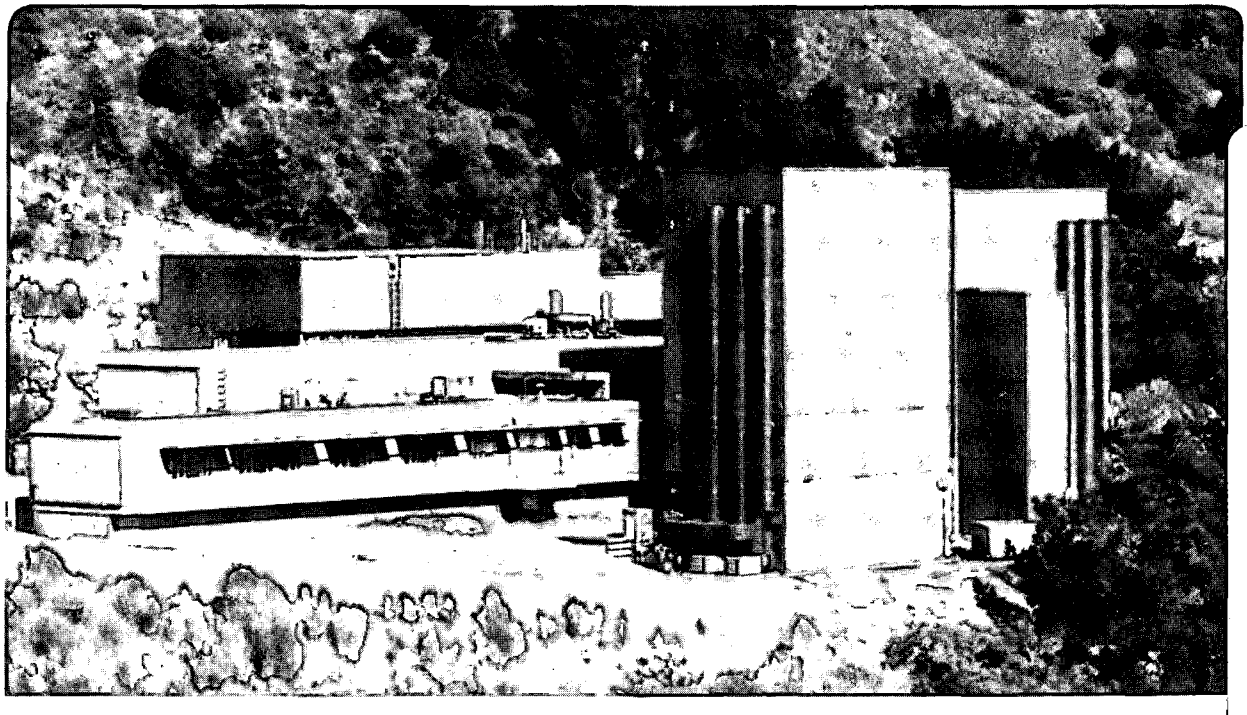
T. Nguyen

July 1991



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

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T. Nguyen

Center for X-ray Optics
Accelerator and Fusion Research Division

and

National Center for Electron Microscopy
Materials Sciences Division
Lawrence Berkeley Laboratory
University of California, Berkeley, CA 94720

and

Department of Materials Science and Mineral Engineering
University of California, Berkeley, CA 94720

Proc. EMSA/MAS Meeting, San Jose, 8/4-8/9/91

This work was supported in part by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Science Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, and by the Air Force Office of Scientific Research, of the U.S. Department of Defense under Contract No. F49620-87-K-0001 through the Center for X-Ray Optics.

HEXAGONAL PHASE IN TENSILE LPCVD POLY-Si FILM

Polycrystalline silicon (poly-Si) films have found many applications in integrated circuits,[1] and in actuators and sensors.[2] Important considerations in the processing of these devices are structural stability and repeatable mechanical properties of the films. The texture and stress state of the films depend strongly on the microstructures and morphology of the films. Tensile films, which are preferred to compressive films in devices whose lateral dimensions of clamped structures are not to be restricted by compressive buckling,[3] are characterized by equiaxial grain morphology, while compressive films are characterized by columnar grain growth during deposition.[4]

A diamond hexagonal (d.h.) Si structure with lattice parameters of a = 3.8Å and c = 6.28Å was first reported in 1963.[5] More recently, transformation from the diamond cubic (d.c.) Si to the hexagonal phase has been observed in Si under hydrostatic pressure at temperatures between 350 C and 700 C,[6,7] in heavily ion-implanted silicon,[8] and in as-grown, implanted, and annealed CVD Si thin films,[9] in addition to the known high pressure Si phases. Pseudopotential calculation showed that the d.h. Si is not a thermodynamically stable phase, and that the structural energy of the d.c. Si is only slightly lower than that of the d.h. Si under atmospheric pressure.[10] The experimental reports seemed to indicate that the transformation resulted from a stress-induced mechanism. It has been shown that the transformation is related to stress relief when twins in f.c.c. or d.c. materials intersect,[11] and that the d.c. to d.h. transformation may be induced by uniaxial compressive and/or tensile stresses.[8] We have, however, observed the d.h. phase in as-grown LPCVD tensile poly-Si films. In this paper, we report the microstructures of, and the presence of the d.h. phase, determined from the extra rings in the cross-sectional electron diffraction pattern, in LPCVD silicon films.

The deposition, and the structural, texture, and stress properties, of the poly-Si films have been reported elsewhere.[5,12] Undoped poly-Si films of thickness 0.5 to 3.5 μm were prepared from pure silane in a front-injection LPCVD reactor. The film in this study is from a zone transition prepared at temperature near 620 C, in which the wafers closest to the has inlet were tensile with equiaxial grains and the last wafers were compressive with columnar grains. Samples for cross-sectional TEM were prepared by mechanical thinning and ion milling in a cold stage,[13] and were examined in a Philips EM 301 operating at 100 kV, or in a JEOL JEM 200CX operating at 200 kV.

Figure 1 is a HRTEM bright-field image of the film, which shows the Si substrate, the 0.1 μm thick silicon oxide layer, and the tensile poly-Si film. LPCVD Si films grown near crystallization temperature initially form an amorphous solid that subsequently crystallizes during the deposition,[14-15] resulting in the equiaxial grains. Amorphous LPCVD silicon films are known to have compressive stress.[16] The transformation from the amorphous state to the crystalline state during deposition results in a volume contraction and hence induces the tensile state in the film. Twins and faulted regions have been observed in the films and at the Si / oxide interface. Figure 2 shows a grain which nucleated near or at the interface. Twin planes are as indicated (T) in the figure. The narrow strip of atomic planes between the arrows has structure different from that of the surrounding [110] silicon, and shows a stacking sequence ABAB... similar to that of hexagonal structure, although first-order twin of the d.c. lattice resulting from shear stress can also results in the same stacking, and formation of twins are more energetically favorable than transformation to the hexagonal phase.[8] It is possible that the twins cross each other and produce a d.h. phase at the intersection, or a twin nucleates inside another twin to produce a long and narrow d.h. region,[7] in such a highly faulted material. However, a larger area of these planes observed is needed for confirmation of it being the d.h. phase, since a few or isolated planes as such can be of faulted d.c. structure.[17]

The presence of the hexagonal phase in the LPCVD tensile poly-Si film is determined from the extra rings in the electron diffraction pattern taken from a large cross-sectional area. The dominant d.c. Si rings, and the extra rings corresponding to the d.h. phase are shown in the figure 3. The most visible hexagonal rings are about the $\{111\}_{d.c.}$ ring, denoted by $\{111^+\}$ and $\{111^-\}$, similar to peaks in x-ray diffraction and rings in electron diffraction patterns reported,[9] and near the $\{311\}_{d.c.}$ ring, or $\{311^+\}$. Rings around $\{331\}_{d.c.}$, however, were not seen probably because of the low intensity of the rings. The inset on the left shows an enlarged section of the $\{111\}_{d.c.}$ ring showing the $\{111^+\}$ and $\{111^-\}$ rings. Measurements from the $\{111^-\}$ ring, or correspondingly $\{100\}_{d.h.}$, and other hexagonal rings yield the values for a and c close to those reported within a few percent. The mechanism for the presence of the d.h. phase in LPCVD tensile Si films, however, is still not understood. It could be one of the mentioned transformation mechanisms from the d.c. structure, or it could nucleate from the amorphous state during deposition. Further studies are needed to understand fully this phenomenom.[18]

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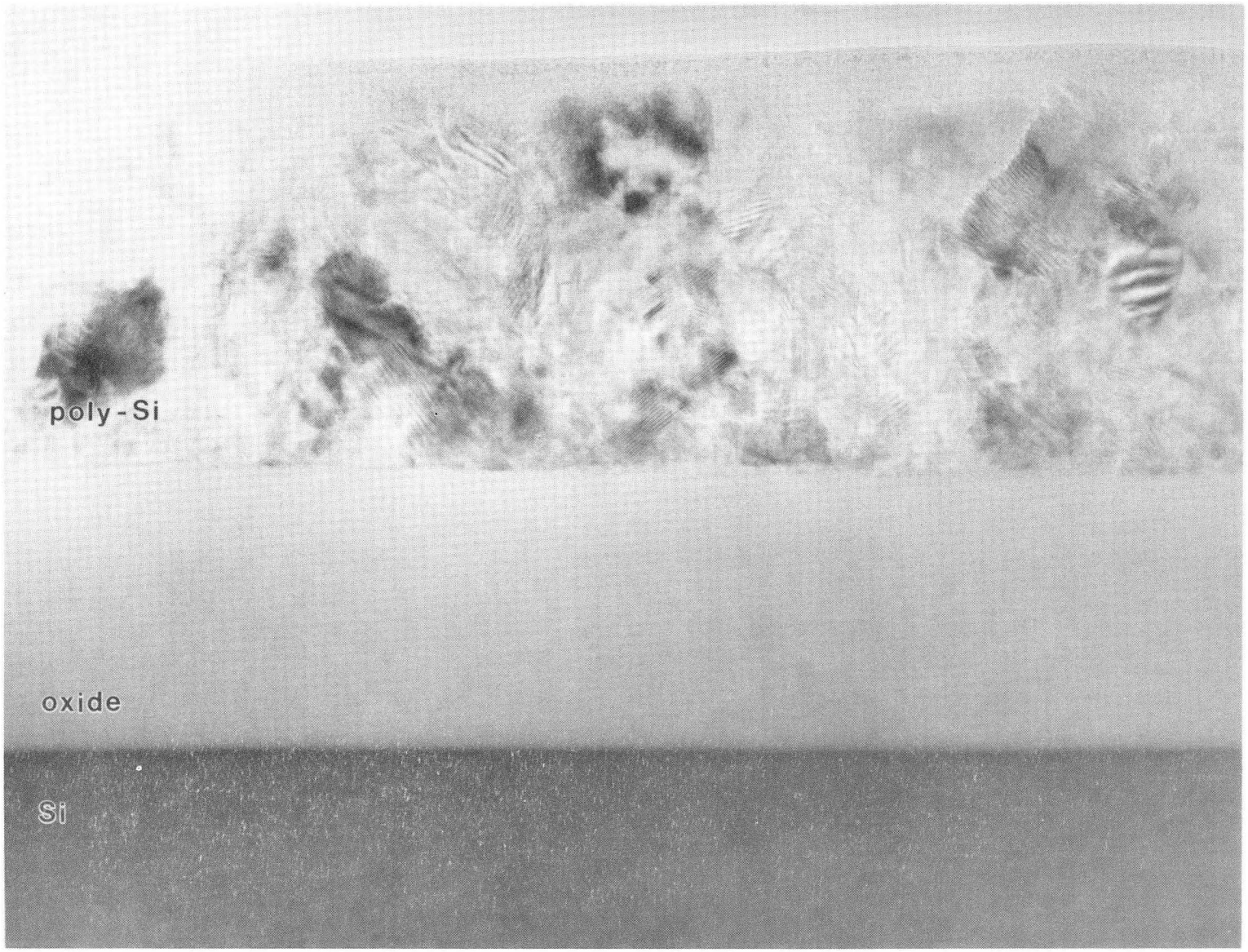

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FIG. 1.--HRTEM bright field image of a as-grown LPCVD tensile poly-Si film.

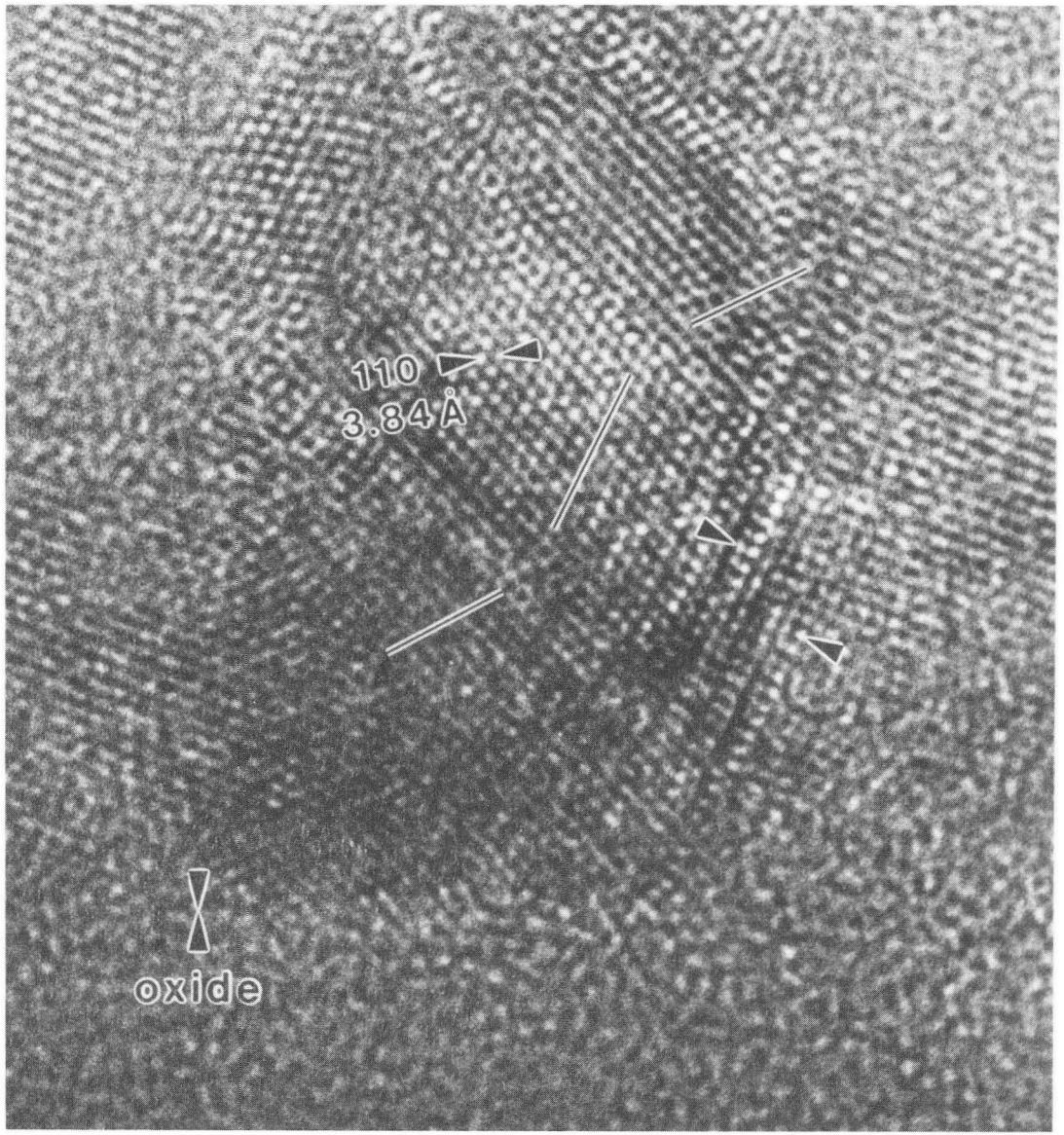

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FIG. 2.--Tensile poly-Si at the Si / oxide interface, showing twins and highly faulted region.

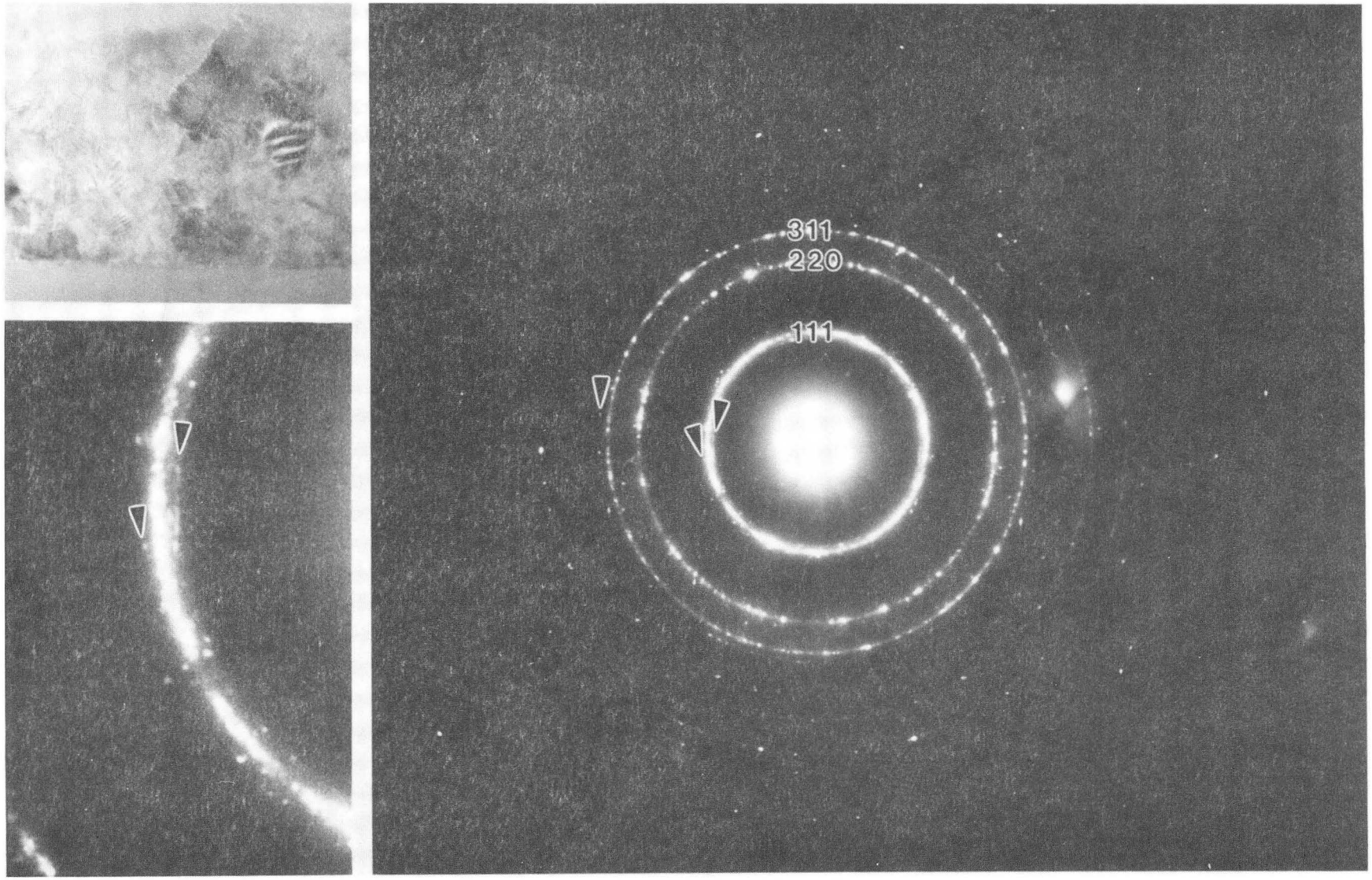

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FIG. 3.--Electron diffraction pattern of cross-sectional sample, showing the d.c. Si and the extra rings corresponding to the d.h. phase. The inset on the left shows an enlarged section of the d.c. {111} ring with the extra d.h. rings.

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INFORMATION RESOURCES DEPARTMENT
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