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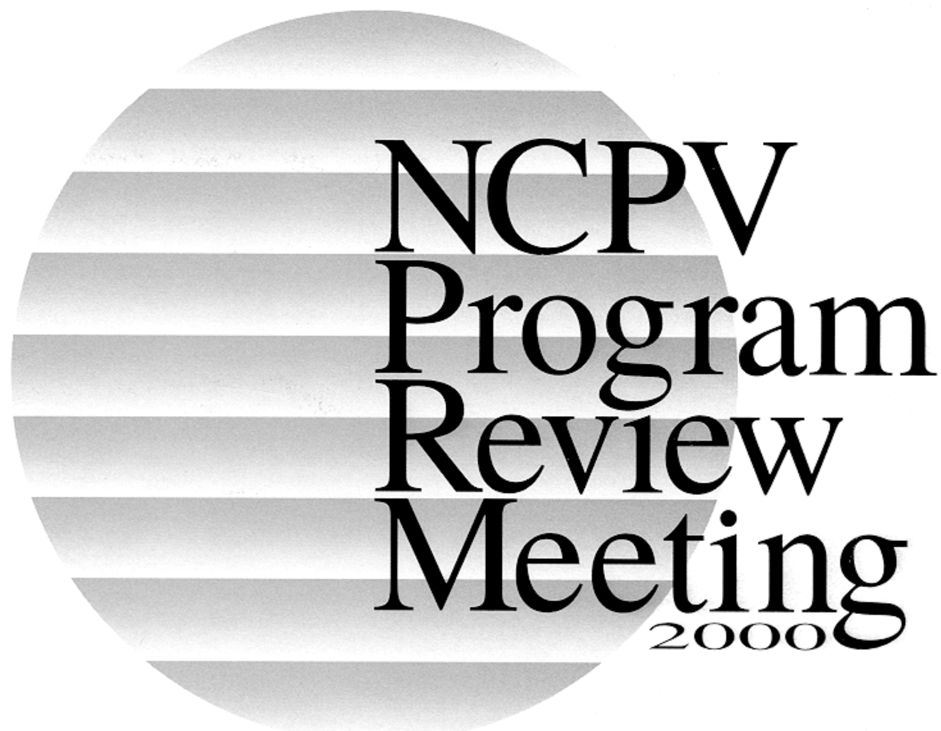

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Structure and Effects of Extended Defects in Polycrystalline Si Thin Films

Y. Yan, M. M. Al-Jassim, T. H. Wang, and T. F. Ciszek

National Renewable Energy Laboratory

1617 Cole Blvd, Golden, CO 80401

ABSTRACT

The structure and effects of extended defects in rapid deposited polycrystalline Si thin films were studied using a combination of high-resolution transmission electron microscopy and first-principles total energy calculations. We found that the extended defects are mainly lamellar twins, and intrinsic and extrinsic stacking faults. The stacking faults were found to attract vacancies and produce energy barriers for oxygen diffusion, while lamellar twins have very little effect on the vacancies and oxygen impurities.

1. Introduction

Recently, high-speed deposition of large-grain polycrystalline silicon thin films on foreign substrates has been achieved using iodine vapor transport of silicon at atmospheric pressure with a vertical thermal gradient [1]. A consequential issue accompanying the high-speed deposition is the formation of a high-density of extended defects in the thin films. It is, thus, important to understand the atomic structure of these defects and their effects on the electronic properties of the films. In this paper we use a combination of high-resolution transmission electron microscopy (HRTEM) and first-principles total energy calculations to study the structure and effects of the extended defects in fast-grown polycrystalline Si thin films.

2. Experimental and theory

The polycrystalline Si thin films studied here were grown by a technique based on iodine vapor transport of Si at atmospheric pressure with a vertical thermal gradient [1]. Cross-sectional specimens were prepared for electron microscopy by first mechanical polishing to ~100 m thickness, then dimpling the central portion of the specimens down to ~5 m. The samples were subsequently thinned to electron transparency using a 4 kV Ar ion-beam at 14° inclination, then cleaned at a lower voltage (1.5 kV). A liquid N_2 cooling stage was used in order to minimize milling damage. HRTEM images were taken on a Philips CM30 microscope with a Cs = 2.0, operating at 300 kV. The image simulations were carried out using the EMS program package [2].

The total energy calculations were carried out using density-functional theory, local-density approximation (LDA) for exchange correlation, ultrasoft pseudopotentials, and plane waves [3]. The energy cutoff for the plane waves was set at 220 eV. We used supercell for defect calculations. Integration over the Brillouin zone was done using the Pack-Monkhost scheme with two irreducible k-points.

3. Results

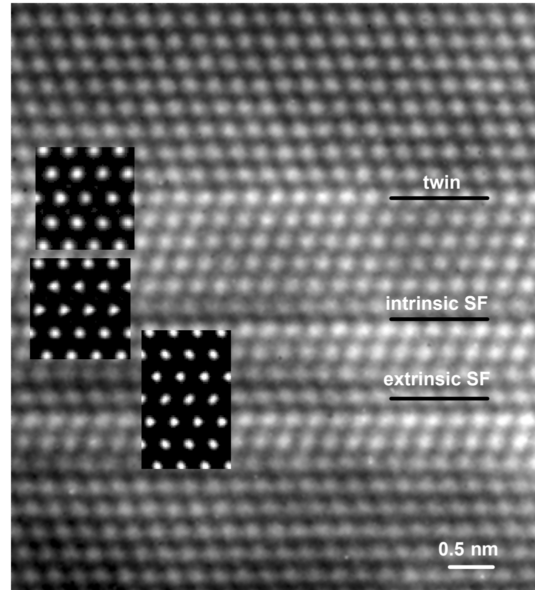

Fig. 1. A $[1\bar{1}0]$ zone axis HRTEM image of lamellar twins, and intrinsic and extrinsic stacking faults in high speed deposited Si films. The insets are the simulated images of the determined structure shown in Fig. 2(b).

Our conventional TEM examinations revealed that the grain sizes of the polycrystalline Si thin films are in the range of 2 to 20 μm. A medium-density of extended defects, mainly planar defects, was observed in most grains.

Detailed analysis revealed that these planar defects are lamellar twins, and intrinsic and extrinsic stacking faults with a habit plane of {111}. The stacking faults often end at a partial dislocation inside the grains. The atomic structures of these defects were determined by HRTEM and image simulations. Figure 1 shows a HRTEM image taken from an area containing the three types of planar defects with the electron beam parallel to the $[1\bar{1}0]$ zone axis. The positions of the defects are indicated by black lines. The characters of the twins and the intrinsic and extrinsic stacking faults are clearly seen from the image.

In cubic materials, the possible structures of lamellar twins, and intrinsic and extrinsic stacking faults lying on {111} planes have been proposed [4]. Figure 2(a), (b) and (c) show the proposed structures for the lamellar twins, and intrinsic and extrinsic stacking faults, respectively. The arrows indicate the positions of the defects. The single and double lines at the defects indicate the bonding configuration across the defects. The open and black circles denote different heights. To demonstrate whether our observed planar defects have the same structure as the proposed, we performed through-focus and through-thickness image simulations. The inserts in figure 1 are the simulated images using the structures shown in figure 2 at a defocus of -60 nm for a thickness of 10 nm. There is no expansion or compression perpendicular to the twin boundary included in the structure. The good fitting demonstrates that the planar defects are indeed twins, and intrinsic and extrinsic stacking faults with the structures as shown in figure 2.

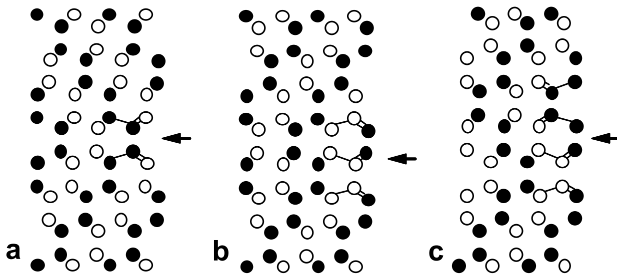

Fig. 2 $[1\bar{1}0]$ projections of the structures of: (a) a lamellar twin boundary; (b) an intrinsic stacking fault; (c) an extrinsic stacking fault.

We now turn to the effects of these planar defects on the properties of the thin films. First-principles calculations have shown that both intrinsic and extrinsic stacking faults produce some very shallow defect states [5]. However, no deep defect states were found. The main reason is that there are no wrong or dangling bonds across these defects. Nonetheless, these structural defects may interact with point defects and thus affect dislocation motion, vacancy migration, and impurity diffusion. Using first-principles total energy calculations, we studied the interaction between the planar defects and vacancies, and oxygen impurities. We first calculated the total energies of supercells containing a vacancy at the defects and at the bulklike region. We found that the formation energy of a vacancy at an intrinsic and an extrinsic stacking fault is lowered by 0.13 and 0.07 eV respectively, compared to that of the crystal site, while a lamellar twin does not change the formation energy. This indicates that stacking faults attract vacancies. Our result of the vacancy at the intrinsic stacking faults is consistent with a recently reported calculation [6].

We then calculated the differences in formation energies of oxygen interstitials in the bulk and at the defects. Oxygen is an important impurity in Si. Oxygen impurites are very mobile at temperatures in the 400 - 500 °C range and can form a family of distinct "thermal" double donor defects. The normal position of an oxygen interstitial in a Si lattice is shown in figure 3. We found that the formation energy of an oxygen interstitial at the intrinsic stacking faults is higher by 0.17 eV than that in the bulk; whereas it is 0.18 eV lower at the extrinsic stacking faults than that in the bulk. This means that intrinsic stacking faults will repel oxygen impurities, but the extrinsic stacking faults will attract oxygen. At the lamellar twin, the formation energy of an oxygen interstitial is only 0.08 eV higher than that in the bulk, indicating less interaction with oxygen impurities.

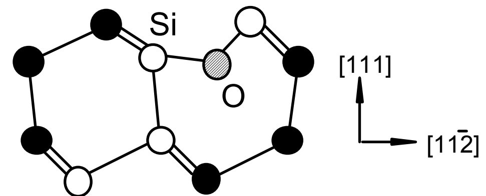

Fig.3 Projection of a Si lattice on a $(1\bar{1}0)$ plane showing the position of an O interstitial.

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