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Carbon at twin-boundaries in multi-crystalline ribbon silicon

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Multi-crystalline silicon (mc-Si) as a low cost material for solar cell applications generally contains impurities and crystal defects with a higher concentration than found in single-crystal Si. The edge-defined film-fed growth (EFG) is a ribbon growth which allows wafer production of high quality with a high output and at low cost [1].

Macroscopically, EFG wafers are characterized by high local mechanical stresses, which are up to five times higher than in other mc-Si materials [2]. TEM investigations demonstrated that in these strained regions a high density of twin lamellae occurred having line densities in the range of 10^3-10^4cm^{-1}. Microtwins, in general, cannot explain the formation of local stresses. This non-uniform stress is not caused by dislocations. Therefore other sources (impurities) have to be taken into consideration. Particularly EFG wafers are highly supersaturated with carbon reaching a concentration of up to 7-10x10^{17}cm^{-3}[3]. However, precipitation of SiC could not be detected by TEM so far.

Our electron optical analysis was carried out on <110> oriented samples with the {111}-twin boundaries parallel to the electron beam (Figure 1). EDX measurements revealed the presence of higher carbon concentration in regions of the microtwins [4]. The question on its local distribution was answered by combining HREM investigations with ab-initio simulations of different interface/defect structures to minimize the total energy of the twin boundary. One of these models describing segregation of C at the twins as used in the simulations is shown in Figure 2 assuming that the C atoms occupy half of the {111}-twin double plane. The relaxation of the pure Si twin (Fig. 2a) results in less than 0.1% bond length rearrangements near the twin, the incorporation of C (cf. Fig. 2b with 2c) yields to a drastic bond length modification. Thus in the energy minimized lattice the distance of the horizontal {111} planes is reduced by 0.5Å near the twin. For comparison with further models and a description of the techniques used in molecular dynamics relaxations cf. Ref. [5]. Such a predicted reduction of the lattice distance was confirmed by measurements of the lattice distance in experimental micrographs. In Figure 3 the twin boundary is marked by T. To measure changes of the perpendicular lying {111} planes, templates of undisturbed Si lattice regions were inserted as shown by the box in the center. On the right side, the fringes of twinned lattice and the undisturbed matrix are aligned by their peaks of fringe intensities. On the left a shift of the {111} fringes of about $\Delta d=0.4\pm0.1$ Å is detectable. This shift is extended over 2 to 3 planes.

Figure 4 shows simulated 400kV-<110>-HREM thickness series for an ideal {111}-Si twin (upper row) and for a C occupied twin boundary (lower row). The twins are indicated by T. The image size is 1.9x1.9nm^2. The simulations demonstrate that imaging conditions exist which reveal the substitutional C in the twin boundary. The detailed analysis, however, separating alternative models and including diffusion and precipitation needs image matching of defocus-thickness series.

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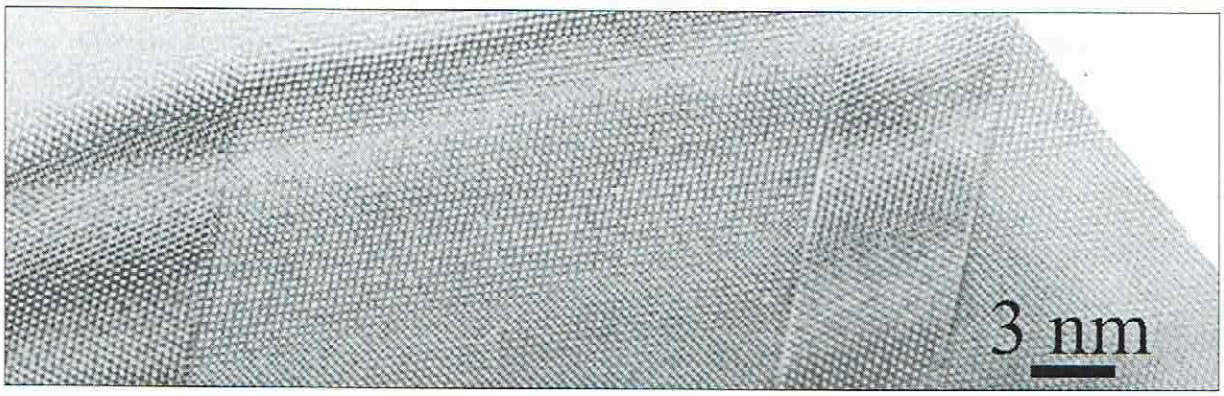

Figure 1. HREM micrograph of a <110> oriented sample with {111} twin boundaries changing their contrast due to the crossing thickness contours.

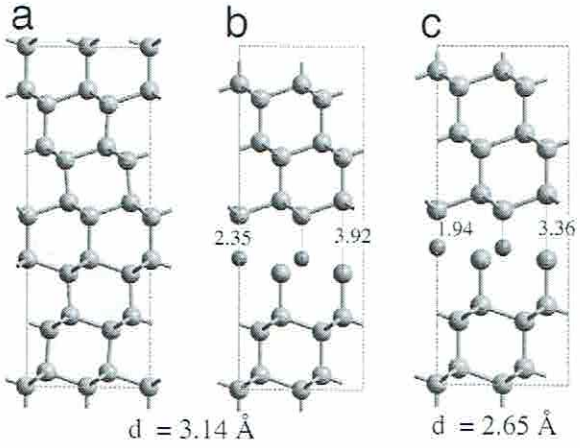

Figure 2. Models for ab-initio structure simulations to minimize the total energy: a) Si twin with an overall {111} lattice plane distance of 3.14 Å. b) half of the twin double plane occupied with C atoms c) relaxed structure with reduced lattice plane distance.

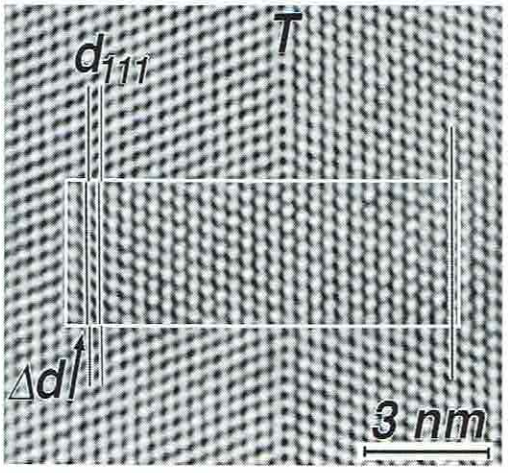

Figure 3. HREM micrograph of a <110> oriented twin boundary T. To demonstrate the reduction Δd of the {111} planes at the boundary, an image of non-disturbed Si matrix is inserted.

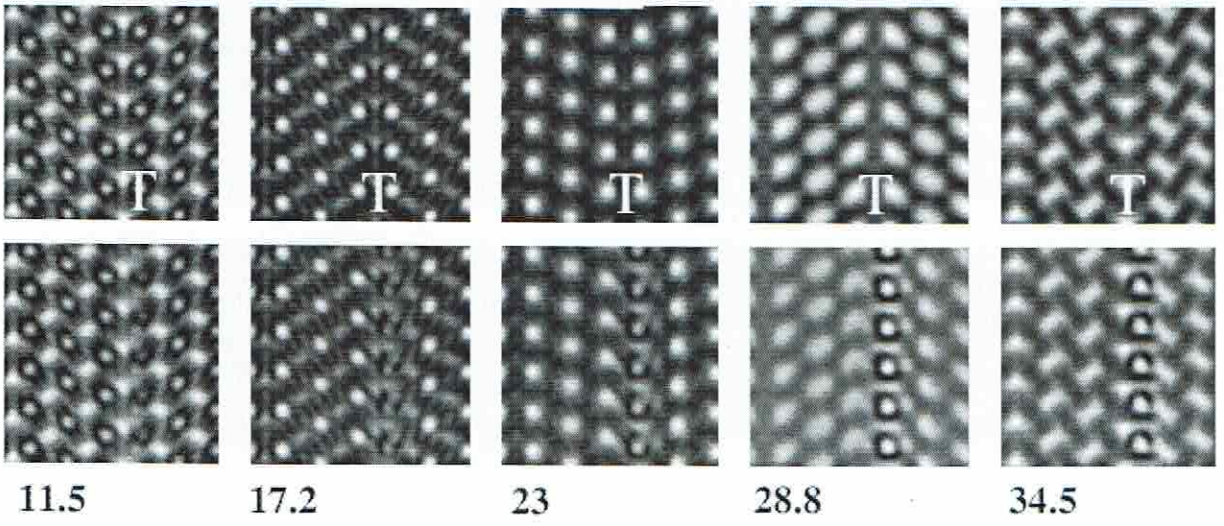

Figure 4. Calculated 400kV-<110>-HREM thickness series (t in nm, Cs=1mm, Δf = 40nm near Scherzer focus, defocus spread 10nm, beam divergence 0.5mrad) for a relaxed ideal {111}-Si twin (upper row) and a twin boundary containing C atoms (lower row).