

Structural Characterization of the Si(111)-CaF₂ Interface by High-Resolution Transmission Electron Microscopy

In a recent Letter¹ Batstone, Phillips, and Hunke (BPH), relying on the interpretation of high-resolution images of cross-section samples by transmission electron microscopy (TEM), claim to have "determined directly" the atomic structure of the Si(111)-CaF₂ interface, although a systematic study of the possible interface geometries was not undertaken: only adsorption of the CaF₂ interface atom on top of a first layer Si atom was considered (i.e., all Si atoms were constrained to fourfold coordination).

Recently Tromp and Reuter (TR) determined the structure of this interface with high accuracy using medium-energy ion scattering (MEIS)²: The interfacial Ca-F layer has lost half of its F atoms; i.e., the Ca/F ratio at the interface is 1. Secondly, Ca bonds to Si with the Ca atoms adsorbed on the so-called *T*₄ site, a threefold site on top of a second-layer Si atom. The second-layer Si atoms are *fivefold* coordinated. The top-site geometry proposed by BPH and the threefold hollow (*H*₃) site do not agree with the MEIS data. The interface structures proposed by BPH and TR are shown in the bottom halves of Figs. 1(b) and 1(c), respectively. The TR interface model is very similar to the bulk structure of CaSi₂ with Si-Ca bond lengths between 3.06 and 3.09 Å. The Si-Ca bond length in the BPH model is between 2 and 2.3 Å. Si-Ca bond lengths in CaSi₂ are 3.03 to 3.06 Å.³

We have performed TEM experiments under conditions similar to those used by BPH, i.e., near Scherzer defocus and with white dots corresponding to channels in the (110)-oriented Si lattice. The microscopes used in this study (Phillips 430 at 300 kV) and by BPH (JEOL 4000EX at 200 kV) have identical contrast transfer characteristics. Epitaxial CaF₂ films were grown at 630°C. A high-resolution micrograph of the Si(111)-CaF₂ interface (Fourier filtered for noise removal and contrast stretched) is shown in Fig. 1(a). The interface is coherent and free of steps over the entire area shown, and high contrast is obtained in both Si and CaF₂. Notice the blurring of the crystal channels at the interface (indicated by the arrow) as opposed to the separate white spots in the Si and CaF₂ lattices.

Since CaF₂ decomposes readily under the electron beam we only took single snapshot images, like BPH, rather than through-focus series. Because micrographs of 3-Å detail are easily obtained in instruments capable of resolving 2.3 Å, nearly optimum contrast transfer is obtained even when micrographs are taken without viewing the area prior to beam exposure. Since the location of the CaF₂-Si interface cannot be determined with certainty in the experimental image, the lateral registry of the CaF₂ and Si lattices can be determined only modulo

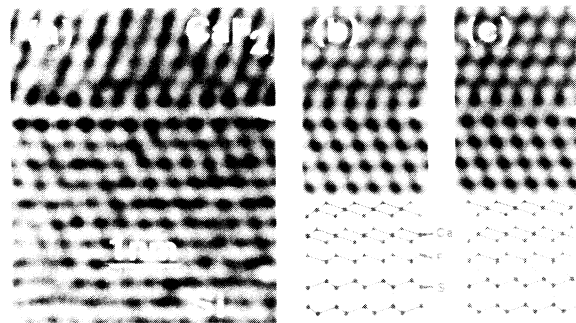


FIG. 1. (a) High-resolution TEM image of the Si(111)-CaF₂ interface. The arrow indicates blurred crystal channels at the interface. (b) Image simulation for the BPH model (shown in inset). (c) Image simulation for the TR model (shown in inset). The arrows in panels (b) and (c) indicate the location of the interface.

2.217 Å from the positions of the channels far from the interface. Therefore, detailed image simulations are needed to establish which model [1(b) or 1(c)] agrees better with the experimental image.

We have performed such image simulations for the BPH and TR models as shown in Figs. 1(b) and 1(c). We find that the BPH model does not agree very well with the experimental image. The TR model, on the other hand, reproduces all the important features of the experimental image. In particular, the blurring of the channels at the interface is very well reproduced in the simulated image [arrow in Fig. 1(c)].

We conclude that there is no conflict between the MEIS results and TEM. The interface structure determined with MEIS [Fig. 1(c)] is fully compatible with TEM observations, whereas the structure shown in Fig. 1(b) is incompatible with both MEIS and TEM data.

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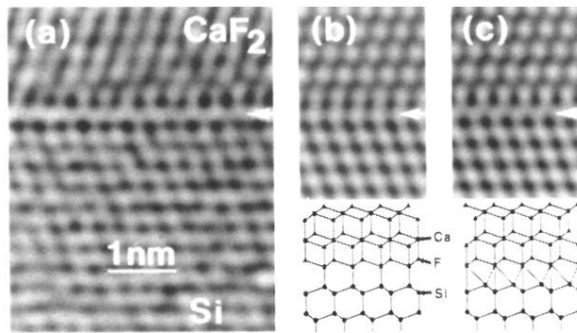


FIG. 1. (a) High-resolution TEM image of the Si(111)-CaF₂ interface. The arrow indicates blurred crystal channels at the interface. (b) Image simulation for the BPH model (shown in inset). (c) Image simulation for the TR model (shown in inset). The arrows in panels (b) and (c) indicate the location of the interface.