# Determining the GaSb/GaAs-(2x8) Reconstruction and Its Impact on Stress Relaxation

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**Motivation**—The critical film thickness of lattice-mismatched heterostructures, such as GaSb/GaAs, is limited to a few mono-layers before 3D islands form. This transition limits the types of devices, such as lasers, detectors, solar cells, and transistors that can be fabricated. Therefore, increasing this critical thickness has been the focus of much recent research. In this work, we focus on understanding the role of surface reconstructions in dislocation formation, because of their ability to relax the misfit stress at the interface and avoid 3-D island growth.

**Accomplishment**—The (2x8) reconstruction of GaSb/GaAs has been reported by the Huffaker group to be associated with nearly complete misfit strain relief through the formation of an array of misfit dislocations at the GaSb/GaAs interface. We examine three possible structures of the (2x8) reconstruction of GaSb for various strain conditions. The first structure was initially proposed for the InSb (2x8) reconstruction, and is referred to here as the α(2x8) (Fig. 1a). The second structure, the β(2x8), (Fig. 1b) is similar, except that it is built from the III-As β2(2x4) reconstruction that contains two Sb surface dimers (outlined in Fig. 1b) and exhibits a similar simulated STM image and line scan. The addition of an extra Sb surface dimer to the backbone results in wider rows along the [110] changing the line scan shape to a cycloid. The third structure was proposed by Laukkanen et al as a possible structure for the GaSb-(2x8) reconstruction. Because this structure also contains the β2(2x4) unit cell as a basis structure, we call it the β2(2x8) reconstruction. The β2(2x8) only has a single Sb dimer in the topmost surface layer, which requires the introduction of Sb atoms into anti-sites in the topmost cation layer to maintain charge neutrality. At the GaAs lattice parameter, our model demonstrated that the stable GaSb/GaAs-(2x8) reconstruction is the α(2x8) or β(2x8) depending on Sb chemical potential. The β(2x8) has a lower energy than the α(2x8) at the InP lattice parameter, but the α(2x8) decreases much more rapidly in energy as the lattice constant is reduced further to become stable at the GaAs lattice parameter. These results also show that the proposed β2(2x8) reconstruction is never stabilized, as it is always >25meV per unit area higher than the stable reconstruction at any Sb chemical potential. This higher energy is likely due to the Sb antisites in the structure. This also agrees with the experimental STM images (Fig. 2), which show no periodic change in intensity along the topmost dimer row as would be expected with an anion dimer every second position. Using this structural information, we were able to investigate the interaction between the α(2x8) and β(2x8) reconstructions and an array of misfit dislocations with an eight lattice constant spacing at the GaSb/GaAs interface. The trench associated with these reconstructions was observed to strongly concentrate the stress in the GaSb films in the underlying region resulting in a strong attraction between the dislocations and the trench. For thin layers, this suggests that the barrier for dislocation nucleation would be greatly reduced consistent with experiments.

**Significance**—In this work we use a combination of experimental and computational techniques to examine the structure of the (2x8) reconstruction of GaSb/GaAs as a function of strain. The resulting structures suggest a mechanism to increase the critical thickness for the islanding transition by providing a pathway for inducing an array of strain relieving misfit dislocations at the GaSb/GaAs interface.

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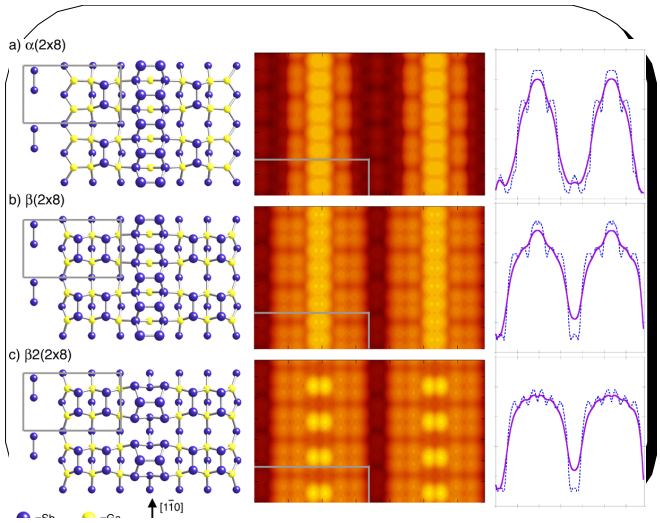


**Figure 1.** Proposed structures for the GaSb/GaAs-(2x8) reconstruction. (a) α(2x8), (b) β(2x8), and (c) β2(2x8). On the left are the atomic structures (Note: Some atoms removed for clarity). In the middle are simulated filled-state (negative bias) STM images. (ticks = 10Å). On the right are line scans of the simulated STM images with the original data (dotted line) and a smoothed line (solid line) calculated using a Steinman function and applying a geometric weighting of the nearest 10% of data points. (x-ticks = 10 Å, y-ticks = 1Å).

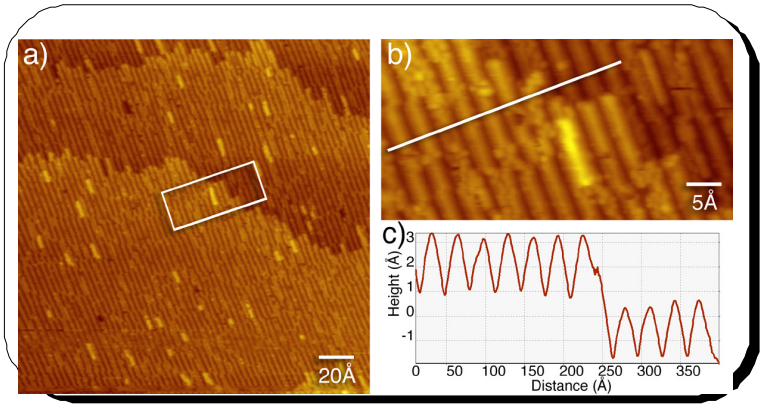


**Figure 2.** (a) STM image (V=-4.07V, I=100pA) of 2.0ML Sb/GaAs cooled under Sb flux to form the (2x8) reconstruction. (b) High resolution portion of the image in (a). (c) A line scan across the line indicated in (b).