Indium-Indium Pair Correlation and Surface Segregation in InGaAs Alloys

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In-In pair correlations and In surface segregation in In Ga_{1-} As alloys are studied by first-principles total-energy calculations. By calculating the substitution energy of a single In atom, we find that the near-surface energetics explains the observed In segregation on InGaAs(001)-$\beta 2(2 \times 4)$ surfaces. Indium surface segregation further enhances the In site selectivity, thus the long-range ordering. We find that the [110] and [001] In-In pair correlations are repulsive and nearly isotropic in bulk but are highly anisotropic near the (001) surface. The sign of the [110] In-In interaction energies vs the distance from the surface is oscillatory. These findings explain the recent puzzling cross-sectional $\times$-STM results.

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Interest in spontaneous ordering [1], composition modulation [2,3], and segregation [4,5]in III-V alloys raised the question of the type of atom-atom interactions that exist at the surface of such alloys. Attractive (repulsive) effective)
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at +59 meV/pair at $= 3$. For $= 2$, however, only the nn pairs involving the strained sites directly under the As-As dimers (i.e., $2c$ and $2c'$) remain repulsive, while others become strongly attractive. Thus, elasticity theory misses the nonmonotonic behavior of J_{nn} while predicting correctly the reversal of the sign of J_{nn} at $= 2$. For $= 1$, $J_{\mathrm{nn}}^{[110]}$ is attractive. To test experimentally the attractive interaction on the $= 1$ surface layer, one needs to perform an *in situ* STM study of the growth surface, not by post-growth $\times$-STM. So far, we are not aware of such a study.

Our results summarized in Table I provide a theoretical