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The reconstructions of Si(15 3 23) TERESA DAVIES, CRISTIAN CIOBANU, Colorado School of Mines — Among the few remaining puzzles in the physics of heteroepitaxial quantum dots, there remains the atomic structure of the facets that bound the dome-shape islands. For a large range of germanium concentrations in the deposited Si- Ge alloy, the (15 3 23) orientation appears to be ubiquitous as the highest-index facet present on the dots at the latest stages of their coherent growth. We present here two approaches to the determination of the reconstructions of Si(15 3 23), one based on a systematic elimination of bonding possibilities and the other being a structural search performed via a genetic algorithm. Both approaches lead to classes of reconstruction models that have much lower surface energies than the only proposal currently available in the literature. Furthermore, the models allow for the presence of low-energy edges between the (15 3 23)-orientations and other facets present on the quantum dots.

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