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Self-organization of atom wires on vicinal surfaces[1]

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Self-organization is possibly the best way to produce nanostructures in large quantities. This also holds for the ultimate 1D system, atom wires; they can be self-assembled in large arrays on vicinal Si surfaces. Such atom wire systems often show intriguing electronic properties such as competing charge density waves and spin-orbit split one-dimensional bands. However, because of their low dimensionality, these wires also frequently show profound thermodynamic fluctuations that limit their *structural* uniformity and have a large influence on their electronic properties. Therefore, in this talk I will focus on structural fluctuations in Ga atom wires self-organized on the Si(112) surface. In these atom wires, strain-relieving adatom vacancies self-organize into meandering vacancy lines (VLs) similar to the well-known nx2 superstructures for Ge on Si(100). The average spacing between these line defects can be experimentally controlled continuously by adjusting the chemical potential μ of the Ga adatoms. Significant VL correlations are discovered in STM experiments that cannot be captured within a mean field analysis. These structural flucuations are well described by a new lattice model that combines Density Functional Theory (DFT) calculations for perfectly ordered structures with the fluctuating disorder seen in experiment, and the experimental control parameter μ. This hybrid approach of lattice modeling and DFT can be applied to other examples of line defects in hetero-epitaxy, especially in cases where correlation effects are significant and a mean field approach is not valid.

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