Complex dynamics and morphologies in nanowire growth

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The vapor-liquid-solid (VLS) process for nanowire growth combines broad technological promise with a captivating elegance. The classic images of VLS growth show slender right prisms of Si growing in the $\langle 111 \rangle$ direction, each neatly capped by a droplet of the Au-Si liquid eutectic catalyst from which it grows. Yet this system is perversely complex, and the classic images are misleading. At high resolution, the Si nanowire sidewalls exhibit a sawtooth texture, contrary to the usual simple picture of VLS growth. Si nanowires are also observed to grow in the $\langle 110 \rangle$ and $\langle 211 \rangle$ directions. These growth modes exhibit a very different structure than $\langle 111 \rangle$, but again one which is contrary to our intuitive picture: the {111}-faceted liquid-solid interface is tilted at an angle to the wire growth direction. The growth direction can be controlled experimentally by the growth conditions (temperature and source-gas pressure), and small changes in growth conditions can trigger kinking from one direction into another.

We show that such complex behavior arises naturally because this system is geometrically frustrated. For Si, the liquid-solid interface is a (111) facet, but there are apparently no stable facets parallel to $\langle 111 \rangle$ for the sidewalls. To have only stable facets, the wire must grow in some more complicated morphology consistent with the available facet orientations [1,2]. In the absence of an obvious simple "best" geometry, there can be multiple geometries that are very different but nearly equally favorable [3,4], and small changes in the growth conditions can tip the balance between them. Such geometrical frustration is common in diamond and zincblende structure semiconductors, because of the dominant role of the (111) facets.

A new theoretical approach [1,2] makes it possible to model the growth of nanowires, and to compare in detail with *in situ* TEM observations [3]. We find a sawtooth morphology, and confirm the role of geometrical frustration. In addition, computer simulations illustrate orientation selection, kinking, and jog formation. Most intriguingly, we find novel oscillatory growth modes. Comparison between simulations and experiments confirms that the simulations capture the most important features of nanowire growth.

This is joint work with K. W. Schwarz

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