Modeling the Growth and Structure of Nanoflags

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The growth and structure of the so-called nanoflag InAs nanowires was studied. These nanowires nucleate from craters on a (001) surface and grow with a pure wurtzite structure along the [0001] axis, inclined to the substrate [1]. Then, by experiencing low temperature and high supersaturation they are forced to kink. The new growth direction induces a change from wurtzite structure with a typically rounded shape to a zinc-blende tapered rectangular nanoplate, which gradually converges into a very thin square tip [2]. The obtained nanowires resemble thus small flags (see Fig.1a). The rectangular shape of the flag with two broad (011) facets enabled careful STM measurements revealing that it hosts an atomicscale superstructure on the (011) surfaces (Fig.1c). Recent theoretical predictions suggest that structures with such features should be very well suited for the search and manipulation of Majorana zero modes. Indeed, the tapered global structure of the nanoflag InAs nanowires and the microscopic superstructure may provide two complementary methods for engineering the Kramer's degeneracy within the vicinity of the chemical potential.

Theoretical analysis of the growth and structure of the InAs nanoflags included first Monte Carlo simulation of the crater formation on the substrate surface. Three dynamical processes: adsorption of the InAs particles, diffusion on the surface, and evaporation and detachment of the particles from different surface sites were taken into account. The Monte Carlo approach was again used to explain the shape and structure of the kinked InAs nanowires. Here, the In adatoms diffused along the surface and can either nucleate, creating clusters, or attach to steps that exist on the surface. It is also assumed that the diffusing particles can easily climb up a step on the surface but that coming back is forbidden. An appropriate change in the attachment and diffusion probabilities allowed to model the shape and crystal structure of the observed in the experiment kinked nanowires, as shown in Fig.1b. Finally, the hypothesis that the patterns observed at the InAs (110) surface of the nanoflags are related to As adatoms, was proven by a minimization procedure within the LAMMPS Molecular Dynamics Simulator Tersoff potential.

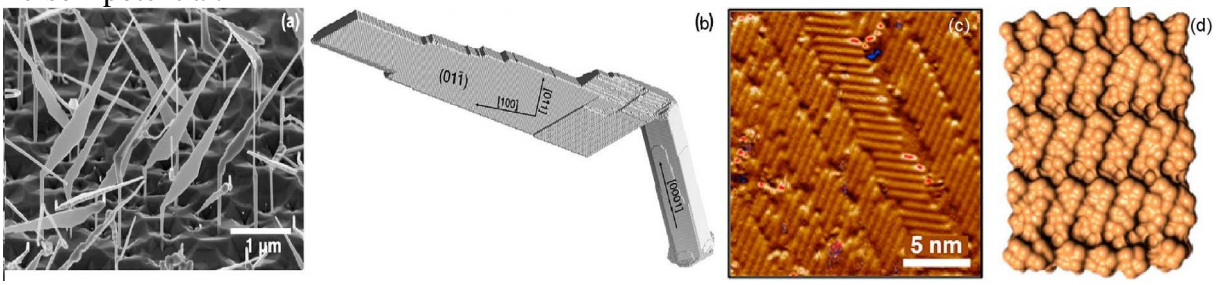

Fig.1. (a) SEM image of kinked InAs nanowires emerging from an InAs (001) faceted surface. (b) The nanoflag nanowire modeled by Monte Carlo simulations. (c) STM topography of the atomic arrangement of the (110) surface of the flag showing 4 unit cell chains arranged in rows. (d) As adatom reconstruction into the superstructure obtained by a minimization procedure within molecular dynamics simulator Tersoff potential transforms.

[1] Jung-Hyun Kang, Filip Krizek, Magdalena Anna Załuska-Kotur, Dr Peter Krogstrup, Perla Kacman, Haim Beidenkopf, Hadas Shtrikman, *Nano Lett.* **18**, 4115 (2018)

[2] M.S. Song, T Koren, M Załuska-Kotur, R Buczko, N Avraham, P Kacman, H. Shtrikman, H. Beidenkopf *Nano Lett.* **21**, 10215 (2021)