Dual-adatom diffusion-limited growth model for compound nanowires: Application to InAs nanowires

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The diffusion-limited model of the growth of nanowires by molecular beam epitaxy, initially developed for silicon nanowires, has been continuously improved over years and extensively applied to describe not only elemental semiconductors, but also compound semiconductors [1]. In the latter case, it assumes either that the growth is limited by one of the constituents (for instance, by arsenic in the case of self-seeded growth of GaAs), or the existence of an "average species" which tries to combine the properties of the two constituents. However, these two constituents may have very different characteristics: A good example is InAs, where arsenic is highly volatile with no or short-ranged diffusion, while indium is not volatile and features a micrometer-sized diffusion length.

In the present approach [2], we calculate the current of adatoms which can reach the nanodroplet and contribute to the growth. Then we assume that the instantaneous growth rate is determined by the minority current. As the current depends not only on the flux from the cell, but also on the nanowire radius and length, the two currents must be calculated for each nanowire of the sample (with its radius) and at each time of the growth (with its instantaneous length). This approach allows us to satisfactorily reproduce the final length of InAs nanowires as a function of the radius (Fig. 1), without changing the material parameters (such as the diffusion lengths) when changing the indium or arsenic flux.

It also reveals several aspects of the growth of compound nanowires, which are expected to apply as soon as the adatoms of the two constituents feature different behaviors - as well-established for III-V compounds, well beyond InAs, and probably true for other, less-known compounds.

- When describing the growth conditions, the flux ratio is not a sufficient criterion. In Fig. 1, the growth of thin nanowires is limited by the arsenic current (due to arsenic evaporation as a result of the Kelvin effect on a volatile species), see Fig. 2a; the growth of thick nanowires is limited by the indium current (due to the strong diffusion of indium adatoms), see Fig. 2c.
- For nanowires with an intermediate radius value, the limiting current switches during growth (Fig. 2b). The switch is abrupt.
- Under steady-state flux conditions, the two maximum currents strongly differ at all times, except for very short periods of time during the growth of certain nanowires, such as at the switching in Fig. 2b. Stoichiometric growth conditions do not exist for a whole nanowire.

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[2] D. Mosiiets, Y. Genuist, J. Cibert, E. Bellet-Amalric and M. Hocevar, Cryst. Growth Des. **24**, 3888 (2024).

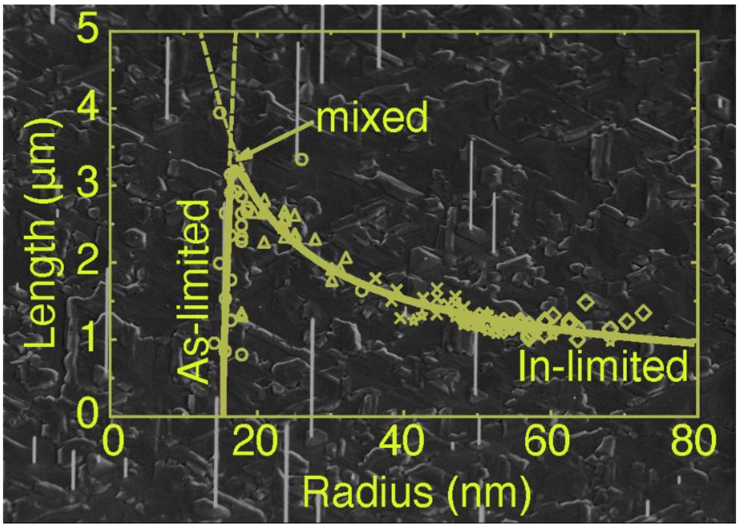

Fig. 1: InAs nanowires: scanning emission microscopy image (background) and length-radius plot. Symbols are experimental, thin dashed lines correspond to the calculated maximum currents of each type, the thick line is calculated using the instantaneous minority currents.

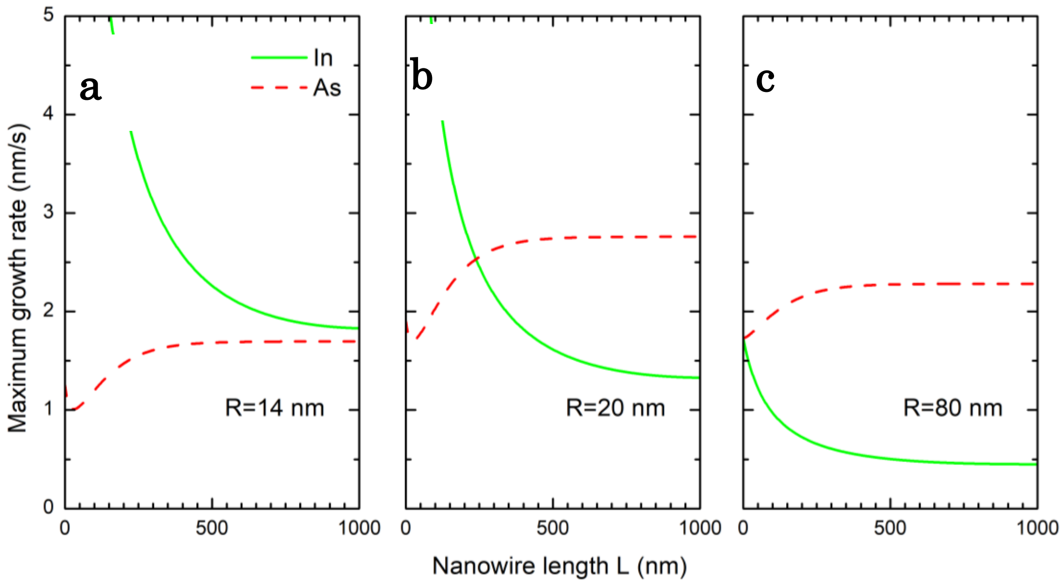

Fig. 2: Calculated indium and arsenic currents (expressed in maximum growth rates of an InAs nanowire), for the growth conditions and fitting parameters used in Fig. 1, as a function of the instantaneous nanowire radius. The arsenic flux impinging the substrate is four time larger than the indium flux. The growth is limited by the arsenic current for a small radius (a, R=14 nm), and by the indium current for a large radius (c, R= 80 nm). At intermediate radius value (b, R= 20 nm), the growth is limited by arsenic at the beginning of the growth, and by indium as the length increases.