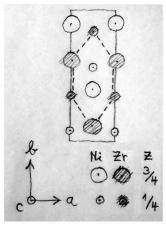
https://spherepacker.github.io/welcome.html

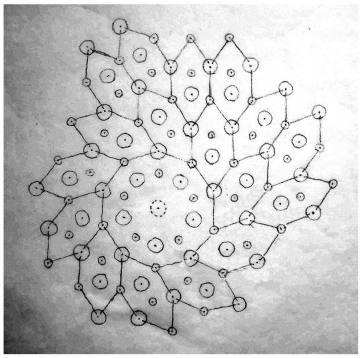
Do We Really Need to See the Atoms?

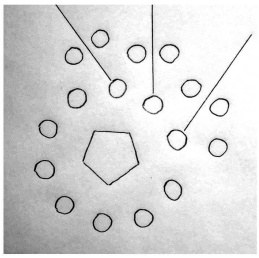
A Counterexample from the Recent Literature



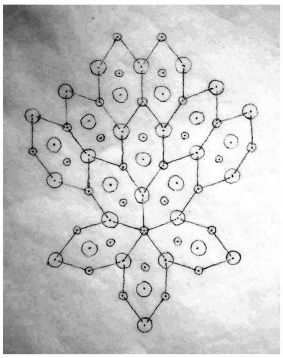
Unit cell of NiZr (orthorhombic) and elongated hexagon used as building unit in the structural drawings on the right.

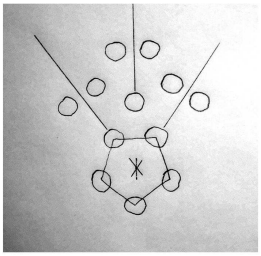
All projections along [001].





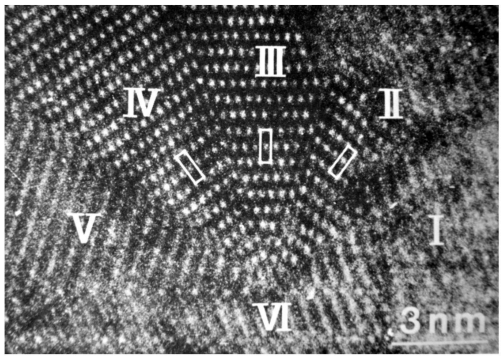
Quasicrystal nucleation according to Hornfeck et al. (2018).

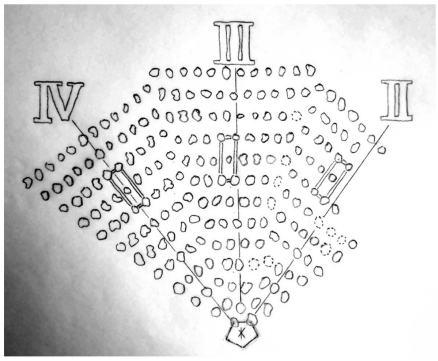




Our proposed alternative model.

In the lower part the circles represent the centers of the elongated hexagons used in the structural drawings at the top. They correspond to the bright spots in the TEM micrograph on the right.





TEM micrograph of NiZr multiple twin by Kuo's group (1985) and its graphical interpretation.

Main points:

- Hornfeck et al. (2018) — *intriguing model* for nucleation and growth of tenfold twins of NiZr (**figure left**) [1].
- Kuo et al. (1985) — observe nucleus of tenfold twin by TEM but *without atomic resolution* (**figure right**) [2].
- Our reinterpretation (2023) — less intriguing (**figure centre**) but the more evident *from Kuo's imperfect data*.

Rationale:

Rows with *equal* numbers of bright spots may be arranged either stepwise (**figure bottom left**) or staggered (**figure bottom centre**). The latter is obviously the case as revealed by experiment (**figure bottom right**).

Résumé:

Hornfeck et al. attempted to prove their atomistic model by means of advanced atomically resolved imaging (HAADF-STEM, high-angle annular dark field scanning transmission electron microscopy). They failed because they did not encounter the tenfold twin's nucleus in their samples. Still they considered their model to be the most likely one. Had they reevaluated the much more imperfect earlier TEM micrograph of Kuo et al. (as we have done now), they would have had to admit that their model is untenable. Thus we see that (a) imagination is more important than advances in imaging and (b) that old literature is still vital. For further details see [3].

[1] *Nature Comm.* **2018**, *9*, 4054.
[2] *Philos. Mag. A* **1985**, *52*, L53.
[3] *https://spherepacker.github.io/welcome.html* — under *References*, items A26 and B15.

Imagination is more important than imaging!