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Do We Really Need to See the Atoms?

M. Petrik[1]

[1] Formerly Philipps-Universität Marburg, Germany

Introduction

Atomic resolution in electron microscopy is almost taken for granted today. In some cases it is regarded as a necessity. – Is imagination and inductive reasoning threatened by blind belief in only what one can see with one's eyes?

Objectives

Employing an example from the recent literature we shall demonstrate that it does not necessarily take state-of-the-art atomically resolved TEM (transmission electron microscopy) to elucidate, say, the structure of a multiple twin of an intermetallic compound on the atomic scale. Less advanced TEM images from as long as forty years ago will do.

Materials and Methods

Wolfgang Hornfeck and colleagues in Dieter Herlach's group recently proposed an intriguing atomistic model for the nucleation of tenfold cyclic twins of orthorhombic (CrB type) NiZr from the melt [1]. They postulated a quasicrystalline nucleus which, when viewed as a 2D projection on a (001) plane, grows in spirals leading to a chiral structure (s. Figure, left). In order to gain further insight, they used HAADF-STEM (high-angle annular dark field scanning TEM) in collaboration with the group of Denis Gratias who also carried out further work on the NiZr twins [2]. In spite of these efforts they were actually unable to produce a TEM image of the tenfold twin's nucleus and, therefore, had to be contented with the mere plausibility of their model which was at least consistent with the atomically resolved structure of the twin boundary.

We asked ourselves in what other ways a tenfold twin might possibly arise given the orthorhombic NiZr structure. By means of pencil and paper and using elongated hexagons of half the volume of the orthorhombic NiZr unit cell as building blocks, we found two other plausible structures, the simpler one of which is depicted here (s. Figure, centre). The representation of these types of structure by elongated hexagons goes back to the group of K. H. Kuo at the Beijing Laboratory of Electron Microscopy in the early nineties [3].

Now, the question is how one or the other of these theoretical twin structures might be experimentally verified.

Results

As pointed out above, the most advanced atomically resolved TEM technique did not yield information on the structure of the tenfold twin's nucleus. We, however, were intrigued by a paper from the group of K. H. Kuo published way back in 1985 [4]. They had succeeded in

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producing a HR-TEM (high-resolution TEM) micrograph of a partially formed NiZr tenfold twin nucleus (s. Figure, right).

Without atomic resolution, using conventional phase contrast HR-TEM under varying defocus conditions, they were able to get an image of the arrangement of the loci of highest electron density which are the centres of the elongated hexagons depicted here (s. Figure).

Conclusion

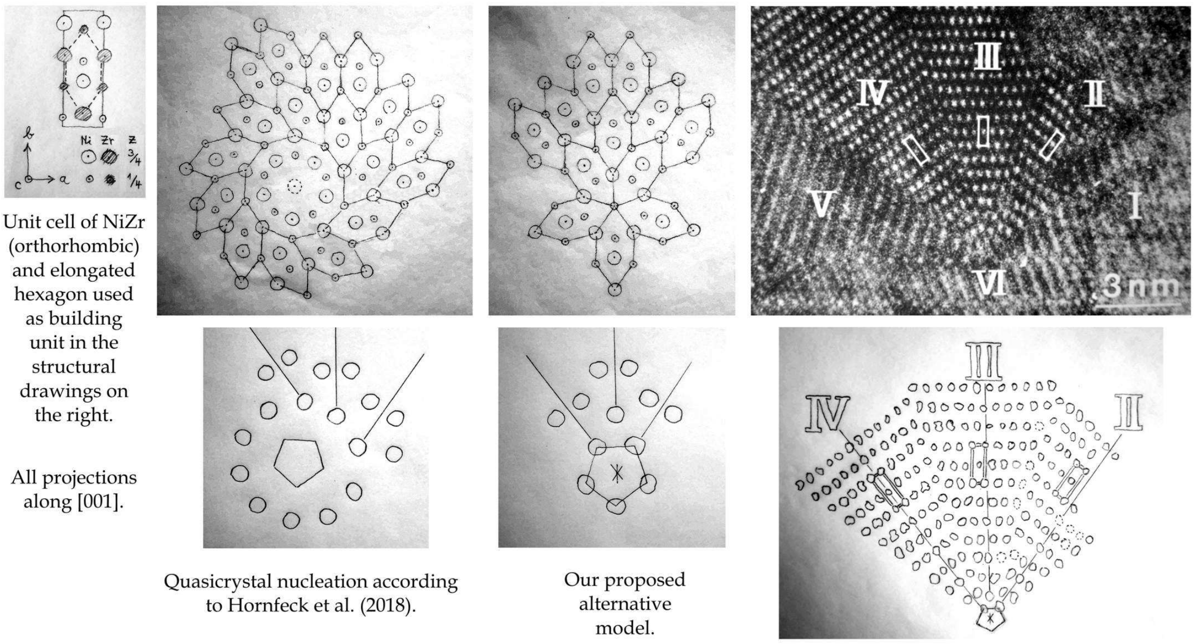
Comparing the three schematic drawings shown (s. Figure, lower parts – solid lines pass along segments' centres), it is seen that the twin structure in the HR-TEM micrograph of 1985 [4] must have been the one proposed here. Only recently did we learn that K. H. Kuo and colleagues had in fact proposed (merely as an aside) the same tenfold twin structure for NiZr already thirty years ago [5].

Lessons learned:

* Imagination is more important than mere imaging.

* Old literature is still vital.

[1] *Nature Comm.* **2018**, *9*, 4054.
[2] *Acta Cryst.* **2018**, *A74*, 647.
[3] *Philos. Mag. B* **1992**, *65*, 525.
[4] *Philos. Mag. A* **1985**, *52*, L53.
[5] *Philos. Mag. B* **1992**, *66*, 117, p. 122.



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.