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Triggering and tracking grain boundary phase transformation at atomic resolution

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Background incl. aims

Phase diagrams and crystallographic defects are essential pillars for modern materials design. In recent years, increasing numbers of defect phases (also known as "complexions") have been identified, and there are evidences on their phase transformations. Nevertheless, due to the vast variety of defects (for example, grain boundaries have five degrees of freedom), it remains challenging to study their thermodynamics in a systematic way, eventually requiring the construction of defect phase diagrams [1].

Methods

We developed a quasi in situ approach to trigger phase transformations of a single grain boundary. The same defect was monitored by atomic-resolution scanning transmission electron microscopy during various steps of triggers. We also developed automatic pattern recognition to distinguish different grain boundary structural units, and applied ab initio simulations to understand their thermodynamics.

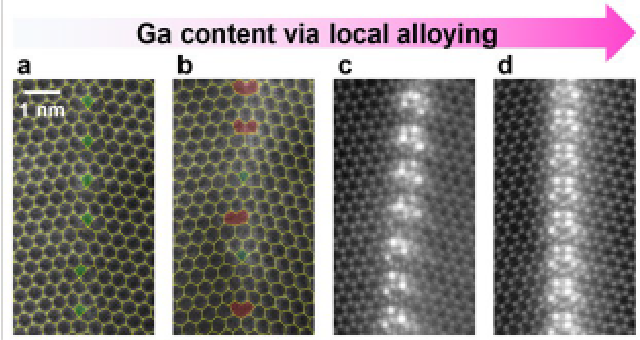
Results

We demonstrate the phase transformation of a Mg grain boundary triggered by local Ga alloying using focused ion beam, as well as the structural evolution with time. As shown in Fig. 1, successive steps of Ga incorporation lead to phase transformations of a Mg [0001] tilt grain boundary [2, 3]. There are two aspects of the phase transformations: 1. Structural transformation from T-type (highlighted in green in Fig. 1a) to A-type (highlighted in red in Fig. 1b) structural units; 2. Formation of chemically ordered grain boundary phases as shown in Fig. 1c, d.

Conclusion

The discovered grain boundary phases and their transformations observed quasi in situ enabled us to construct a phase diagram for this grain boundary. Our developed methodology including atomic resolution imaging, automatic pattern recognition, and ab inito simulations formulates a blueprint to develop defect phase diagrams systematically and propel a new paradigm for materials design.

Graphic:



Keywords:

Grain boundary complexion, phase transformation

Reference:

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