IN SITU TRANSMISSION ELECTRON MICROSCOPY STUDY OF NANOMECHANICAL DEFORMATION AND ATOMIC-SCALE FRACTURE IN HIGH ENTROPY ALLOYS

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Abstract
Intergranular fracture plays an important role in polycrystalline materials including high entropy alloys, but the atomic scale fracture mechanisms of individual grain boundaries (GBs) are still not fully understood. In this work, we selectively investigate the fracture behaviors of individual GBs in a single-phase face-centered cubic CoCrFeNi high entropy alloy via in situ transmission electron microscopy (TEM) nanomechanical testing supported by molecular dynamics (MD) simulations. With this set up, the classic mode I crack propagation along GBs can be dynamically visualized and quantitatively analyzed.

1. Introduction

In contrast to the interaction of a crack with a GB, the intrinsic resistance to crack growth along a given GB often remains elusive. In this work, we use the coherent twin boundary (CTB, an important element of GB engineering) as an example to clarify the propagation of mode I crack along the boundary plane, taking advantage of in situ nanomechanical testing. Custom-designed thin film samples containing a longitudinal TB were fabricated with focused ion beam (ZEISS Crossbeam 540) and in situ nanomechanical testing was carried out in TEM (JEOL ARM300F) equipped with an X-Nano TEM holder. As shown in Fig. 1, the specially designed sample with a preset crack can convert the longitudinal indentation into tensile loading perpendicular to the TB at a strain rate of approximately 10^{-2} s^{-1}. Upon tensile loading, the intergranular crack growth, crack tip opening distance and the associated plastic deformation mechanisms ahead of the crack tip were simultaneously collected and analyzed, which were compared with those in pure copper.

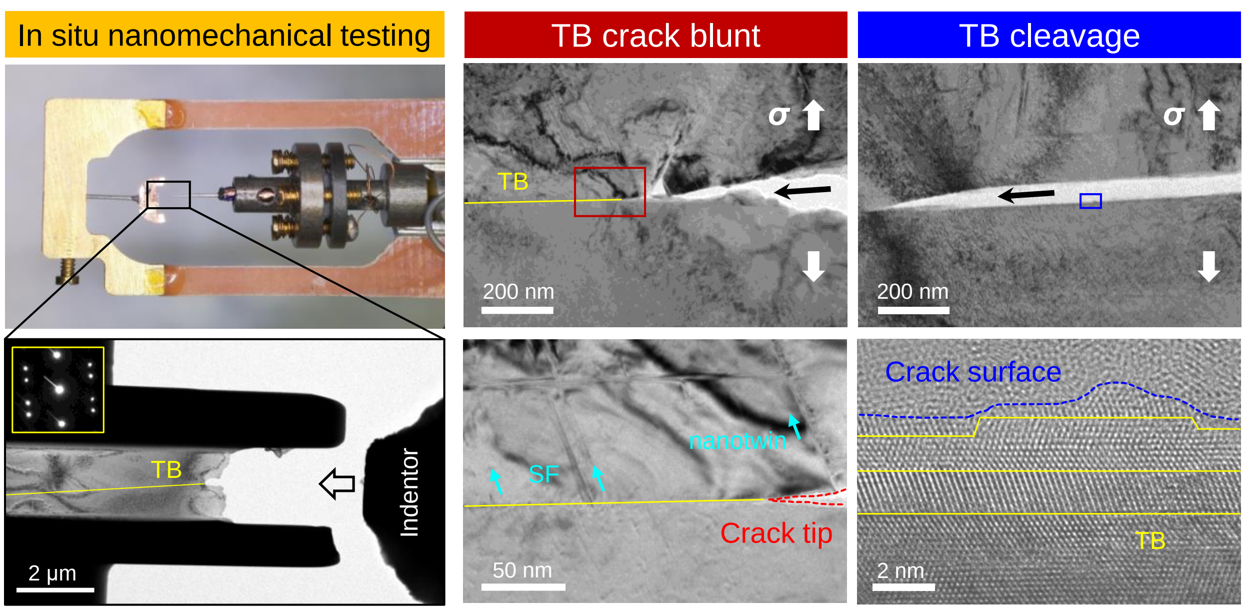

Fig.1 Experimental setup of in situ TEM nanomechanical testing and examples of different fracture behaviors of mode I crack along the TBs in CoCrFeNi high entropy alloy.

2. Results

Taking advantage of the atomic scale resolution of in situ nanomechanical testing, both mechanistic and quantitative understandings of fracture behaviors along the CTB were obtained:

a. An anisotropy of ductile and brittle fracture of the CTB along reversed <112> direction has been revealed in CoCrFeNi alloy, which is dominated by stacking fault (SF)/nanotwin emission ahead of the crack and rapid TB cleavage, respectively.
b. The increasing density of TBs (*i.e.*, nanotwins) tends to constrain the release of elastic strain ahead of the crack tip via dislocation nucleation, thereby favoring brittle fracture along the TB (Fig. 1).
c. A correlation between the stress intensity factor K_I and crack growth along the TB under constant tensile loading rate can be established.

3. Conclusions

Combined in situ TEM nanomechanical testing and MD simulations provides a method to decouple the fracture behaviors of individual GBs from those of GB networks in polycrystalline materials. This method allows a kinetic perspective of GB fracture down to the atomic scale, as opposed to the pure energy perspective of decohesion and interfacial energy. Besides, this method also provides new possibilities to explore mixed-mode crack growth behavior along and across the GBs, which can enrich our understanding of fracture mechanics alongside the classic continuum theory and hold significant implications to GB engineering.

Acknowledgements

The authors acknowledge the Facility for Analysis, Characterisation, Testing and Simulation, Nanyang Technological University, Singapore, for the use of TEM and FIB, and the assistance of Prof. Hongtao Wang from Zhejiang University, China, for technical assistance. SS and HG acknowledge support of this work from their respective Distinguished University Professorships.