

The Hong Kong University of Science and Technology

Department of Mathematics

Seminar on Applied Mathematics

An Upscaling Strategy for Capturing Radiationinduced Grain Boundary Behaviour

by

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<u>Abstract</u>

In this talk, an upscaling strategy is proposed to summarise the microstructural evolution of materials for their long-time macroscopic behaviour, and an example will be shown. Materials containing a high proportion of grain boundaries offer significant potential for the development of radiation-resistent structural materials. However, a proper understanding of the connection between the radiation-induced microstructural grain boundary behaviour and its impact at long natural time scales is still missing. To bridge this gap in time scales, a rigorously coarse-grained formulation describing the coupled evolution of point defects and low-angle tilt grain boundaries is proposed. The derived formulation captures well the radiation-induced climb behaviour of grain boundary dislocations, which leads to asymmetry in grain shape evolution. It also reveals that the presence of point defect sources within a grain further accelerates its shrinking process, and radiation tends to elongate the twin boundary sections. Based on the proposed formulation, it is predicted for the first time that the minimum dimension of a polycrystalline aggregate needed for shielding the point defect concentration to a prescribed level scales with its grain boundary fraction at a sublinear rate. The upscaling strategy used for studying the coarse-grained behaviour of other material systems is also discussed.

References:

Y. C. Zhu, J. Luo, X. Guo, Y. Xiang, S. J. Chapman. Role of grain boundaries under long-time radiation, Phys. Rev. Lett., 120, 222501-5, (2018).

Date: Time: Venue: Monday, 6 August 2018 3:00p.m. – 4:00p.m. Room 5504, Academic Buildings (Lifts 25, 26), HKUST All are welcome!