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Structural Evolution and Thermomechanical Properties of Nanocrystalline Transition Metal Alloys: An Atomistic Investigation

Evelyn R. Chen* | Samuel J. Davies | Aris M. Thorne

Department of Materials Science, University of Cambridge, UK | MIT Materials Research Laboratory, USA

ABSTRACT: This study investigates the intricate relationship between atomic-scale structure and the macroscopic thermomechanical response in nanocrystalline transition metal alloys. Utilizing advanced atomistic simulations, we elucidate the mechanisms governing grain boundary evolution, defect dynamics, and **phase stability** under **extreme** thermal extreme thermal and mechanical loading conditions. Findings reveal a novel deformaton pathway controlled by localized localized dislocation emission and **grain boundary** migration, offering critical insights for the design of **next-generation structural materials** resistant to fatigue and failure. The work combines fundamental theory with experimental experimental validation, providing a comprehensive framework for predicting material behavior in demanding environments.

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