Johns Hopkins University
Department of Mechanical Engineering
2021 Spring Virtual Seminar Series: Class 530.803

Thursday, April 15, 2021 | 3:00 PM – 4:00 PM
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"Mechanism of Enhanced Ductility in Mg Alloys"

Presented by Professor William Curtin

W. A. Curtin[a] , Zhaoxuan Wu[b], Rasool Ahmad[a], and Binglun Yin[c]

[a] Institute of Mechanical Engineering, École Polytechnique Fédérale de Lausanne,

[b] Dept. of Materials Science, City University of Hong Kong

[c]Dept. of Materials Science, Zhejiang U., China

Pure Mg has low ductility due to strong plastic anisotropy and due to a transition of <c+a> pyramidal dislocations to a sessile basal-oriented structure [1]. Alloying generally improves ductility; for instance, Mg-3wt.%RE (RE=Y, Tb, Dy, Ho, Er) alloys show relatively high ductility [2], and typically larger than most commercial Mg-Al-Zn alloys at similar grain sizes. Possible concepts for ductility in alloys include the reduction of plastic anisotropy due to solute strengthening of basal slip, the nucleation of <c+a> from basal I1 stacking faults, the prevention of the detrimental <c+a> transformation to sessile structures, and the weakening of strong basal texture by some solute/particle mechanisms. Experiments and modeling do not strongly support these concepts, however. Here, we introduce a new mechanism of pyramidal cross-slip from the lower-energy Pyr. II plane to the higher energy Pyr. I plane as the key to ductility in Mg and alloys [3]. Certain alloying elements reduce the energy difference between Pyr. I and II screw dislocations, accelerating cross-slip that then leads to rapid dislocation multiplication and alleviates the effects of the undesirable pyramidal-to-basal dissociation. A theory for the cross-slip energy barrier is presented, and first-principles density functional theory (DFT) calculations, following methods in [4], are used to compute the necessary pyramidal stacking fault energies as a function of solute type for many solutes in the dilute concentration limit. Predictions of the theory then demonstrate why Rare Earth solutes are highly effective at very low concentrations, and generally capture the trends in ductility and texture evolution across the full range of Mg alloys studied to date. The new mechanism is used to guide alloy design for achieving enhanced ductility across a range of non-RE alloys [5].

Professor William Curtin earned a 4 yr. ScB/ScM degree in Physics from Brown University in 1981 and a PhD in theoretical physics from Cornell University in 1986. He worked as staff researcher at British Petroleum until 1993 and then joined Virginia Tech as an Associate Professor in both Engineering Mechanics and Materials Science. In 1998 he returned to Brown as Full Professor of Engineering in the Solid Mechanics group, where he was appointed Elisha Benjamin Andrews Professor in 2006. He joined Ecole Polytechnique Federale de Lausanne as the Director of the Institute of Mechanical Engineering in 2011 and officially as Full Professor in 2012. His research successes include predictive theories of optical properties of nanoparticles, statistical mechanics of freezing, hydrogen storage in amorphous metals, strength and toughness of fiber composites, dynamic strain aging and ductility in lightweight Al and Mg metal alloys, solute strengthening of metal alloys including high entropy alloys, and hydrogen embrittlement of metals, along with innovative multiscale modeling methods to tackle many of these problems. Professor Curtin was a Guggenheim Fellow in 2005-06, was Editor-in-Chief of *"Modeling and Simulation in Materials Science and Engineering"* from 2006-2016, has published over 300 journal papers that have received over 19000 citations with an h-index of 75 (Google Scholar), and has been the Principal Investigator on over $37M of funded research projects.

[1] Z. Wu, W.A. Curtin, *Nature* 526 (2015) 62-67
[2] S. Sandlobes, et al., *Acta Materialia* 59 (2011) 429-439; *Acta Materialia* 70 (2014) 92–104
[3] Z. Wu, R. Ahmad, B. Yin, S. Sandlobes, and W. A. Curtin, *Science* 359, 447-452 (2018).
[4] B. Yin, Z. Wu, and W. A. Curtin, *Acta Materialia* 136 (2017) 249-261.
[5] R. Ahmad, B. Yin, Z. Wu, and W. A. Curtin, *Acta Materialia* 172 (2019) 161-184.