Abstract Submitted
for the SHOCK17 Meeting of
The American Physical Society

Spall failure of ultra-high purity single crystals SARA ADIBI, JUSTIN WILKERSON, University of Texas at San Antonio — Spall failure of metals is governed by void nucleation, growth, and coalescence. Recent experimental observations suggest that under extreme conditions nano-void nucleation may be mediated by vacancy clustering in addition to the more traditional view of void nucleation at second phase particles. Here, we use molecular dynamics simulations as a tool to investigate the time-dependence associated with vacancy clustering in ultra-high purity single crystals. The time evolution of the vacancy cluster size statistics are investigated as a function of temperature, pressure, and vacancy concentration. It is shown that increasing the temperature and/or initial vacancy concentration can accelerate the incubation time for generating a cluster of a critical size. Since the critical stress to grow these nano-voids is strongly size-dependent, an interesting time-temperature-vacancy concentration coupling may arise in spall failure. We propose a continuum theory for this diffusion-fracture coupled process, which is shown to provide favorable agreement with our molecular dynamics simulations. This atomistically-informed theory of void nucleation may be integrated into multiscale frameworks of ductile fracture of metals to predict the macroscopic implications of these atomistic processes.

Justin Wilkerson
University of Texas at San Antonio

Date submitted: 23 Feb 2017 Electronic form version 1.4