MATERIALS ENGINEERING SEMINAR

"Role of Dislocations on Martensitic Transformation and Microstructure through Molecular Dynamics Simulations"

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Purdue MSE MS Final Exam

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ABSTRACT

Austenitic to martensitic transformation underlies the phenomena of super-elasticity within shape memory alloys and the production of advanced steels. Experiments and simulations have demonstrated that this process is strongly influenced by defects and microstructure. Molecular dynamics simulations have revealed the atomic mechanisms underlying the impact of grain-boundaries and precipitates on the solid-to-solid phase transformation. Yet the role of dislocations on the martensitic transformation and its microstructures remains unclear.

Therefore, we utilize large-scale molecular dynamics (MD) simulations to study the forward and reverse transformation of martensitic material modeled after $Ni_{63}Al_{37}$ shape via thermal cycling loading. The simulations indicate that dislocations retain martensite well above the martensite start temperature and behave as nucleation sites for the martensite. We found that a reduction in dislocation density with cycle correlated with a decrement in the M_s and A_s transition temperatures, in agreement with experimental observations. It was found that competing martensite variants could develop into stable domains for relatively low dislocation densities that resulted in multi-domain structures. We extracted a critical nuclei size for the martensitic variants.

Date: Tuesday, July 18, 2023
Time: 12:00 P.M. (Noon)
Place: ARMS 1028 or
via this link:https://purdue.webex.com/webappng/sites/purdue/dashboard/pmr/strachan

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