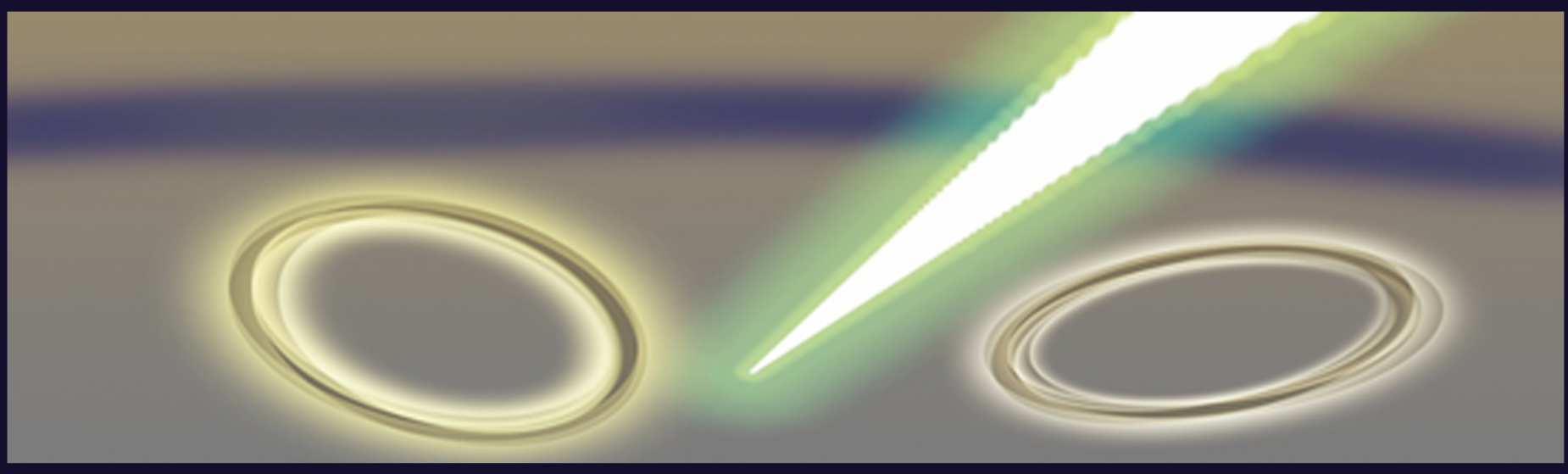

Mystery of the formation of <100> loops in irradiated iron

Dislocations are one-dimensional defects and play an essential role in properties of crystalline, including bcc iron. The <100> interstitial-type dislocation loops commonly exist in irradiated ferritic steels as discovered by Transmission Electronic Microscopy studies since early 1960s. The formation mechanism, however, is still a puzzle despite extensive investigations and debates in the past half-century. It is well accepted that the formation energies for <100> interstitial loops are higher than that of <111> interstitial loops. As a consequence, the <100> interstitial loops are unlikely to form since it is energetically unfavorable. The direct observations of the formation of <100> interstitial loops are therefore absent. Part of the reason is that the generation of these loops are too short for experiments, but also thought to be too long for atomistic simulations. Using large scale molecular dynamics simulations with up to 220 million atoms, we directly observed the dynamical process of the generation of the <100> interstitial loops in a single displacement cascade event. The formation mechanism of these loops will be further discussed, as reported in Ref [1].

[1] Q. Peng, et al., "Shockwave generates <100> dislocation loops in bcc iron", Nature Communications, (2018), 9, 4880 .*

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Virtual Colloquium
3:30 to 4:30 p.m. Eastern Time (U.S. and Canada)
Wednesday, September 9, 2020

See sc.fsu.edu/news-and-events/colloquium for details