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Atomistic shock simulations in defective metals

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I will present molecular dynamics (MD) simulations of shocks in embedded atom method (EAM) metals with pre-existing defects. Samples with prismatic loops and voids have been studied, and analytic dislocation-based models have been used to accurately predict their Hugoniot elastic limit. On the other hand, understanding of nanocrystalline samples is more challenging. Nanocrystals are of great interest due to a number of unique properties, including higher strength and hardness than larger polycrystaline materials. I will show simulations of shock waves in nanocrystals, where grain boundary sliding is reduced and "harder" nanocrystals are observed. Related shock-recovery experiments (details presented in another talk) are being carried out at LLNL, and could open up new applications for nanocrystalline materials. *Numerous people contributed to this work, especially A. Caro and M. Victoria. The work at LLNL was performed under the auspices of the U.S. Department of Energy and Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48, LDRD 04-ERD-021.