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Plasticity and energy absorption at the nanoscale: kinetics and chemical control MATTEO COCOCCIONI, GERBRAND CEDER, NICOLA MARZARI, Department of Materials Science and Engineering and Institute for Soldier Nanotechnologies, MIT — Shock-induced phase transitions of group-IV nanoparticles are investigated using first-principles molecular dynamics in the electronic-enthalpy formalism [1]. In some of these systems a shock compression can induce plastic deformations, leading to to the absorption of the mechanical energy coming from the impact. Kinetic factors greatly affect phase transformations, and so only some of the thermodynamically stable structures are explored. Still, transitions are always nucleated in the core of the nanoparticles, and are accompanied by the formation of small close-packed clusters of characteristic shape. Also, as the particle's size grows, amorphization remains confined in the core region. Finally, we highlight how chemical doping can be used to affect nucleation, and to tune pressure thresholds; this could be relevant e.g. for target applications such as the design of novel impact-absorbing nanostructured materials.

[1] M. Cococcioni, F. Mauri, G. Ceder and N. Marzari, PRL (2005).

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