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MD simulation of Deformation and Fracture in Nanocrystalline Ag and Nano-composite AgNi YUE QI, YANG-TSE CHENG, General Motors R&D — The deformation and fracture mechanisms of columnar nano-crystalline Ag and nano-composite AgNi have been studied using molecular dynamics. In addition to dislocation-mediated plasticity at an early stage of deformation, we found grain-rotation induced grain growth and crack formation at larger deformation. The crack nucleation at the grain boundaries and the linkage of such cracks will finally lead to the fracture of the material. However, the ductility of the nanocrystals is largely controlled by the competition between grain growth and crack nucleation. As a result, lower temperature, larger grain size and introduction of a second phase tend to accelerate crack formation and reduce the fracture strain, such decrease the ductility of the nanocrystals.

Yue Qi
General Motors R&D

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