Deformation and Damage in Structurally Graded Nano-Crystalline Aluminum Alloys

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Structurally graded nano-crystalline (SGNC) materials are a new class of metallic materials that offer the promise of obtaining previously unachievable combinations of strength, ductility and toughness. Structurally graded nano-crystalline materials consist of two or more layers in which the grain size varies from relatively fine (nanometers (nm) or tens of nm) to relatively coarse (hundreds of nm or a few microns). The structurally graded architecture is believed to mitigate the mechanisms that lead to poor ductility and low toughness in traditional nano-crystalline materials; those that have resulted in the inability to exploit the extremely high strength potential offered by nanocrystalline grain structures.

In the present work, computational materials methods are developed to enable microstructural design of SGNC aluminum and similar materials. Atomistic simulation and a new multiscale modeling methodology are used to interrogate microstructures having grains near the lower range of SGNC grain sizes (20 nm to 100 nm) and near the upper range of SGNC grain sizes (100 nm to 2 microns), respectively. The atomistic simulation is based on the embedded atom method (EAM) and uses the Mishin-Farkas potential for aluminum. The multiscale modeling method has been developed as part of this award and combines the predictive capability of discrete dislocation plasticity with the computational efficiency of continuum crystal plasticity as part of the overall design methodology for analysis of larger-grained microstructures.

Although this Phase I investigation is focused on computational evaluation, the state-of-the-art in processing and experimental characterization is also evaluated to determine the feasibility of producing and characterizing these materials. Several possible methods for production of graded materials are assessed for their ability to control grain growth, develop very fine-grained structures and produce appropriate grain size gradients. Additionally, the state-of-the-art in quantitative microscopy, as needed to validate the simulations and characterize deformation and damage modes in these materials, is assessed.