SUPERELASTICITY AND MICACEOUS PLASTICITY OF THE NOVEL INTERMETALLIC COMPOUND $CaFe_2As_2$ AT SMALL LENGTH SCALES

John T. Sypek, University of Connecticut, USA
john.sypek@uconn.edu
Christopher R. Weinberger, Colorado State University, USA
Paul C. Canfield, Ames National Laboratory & Iowa State University, USA
Sergey L. Bud'ko, Ames National Laboratory & Iowa State University, USA
Seok-Woo Lee, University of Connecticut, USA

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Shape memory materials have the capability to recover their original shape after plastic deformation when they are subjected to certain stimulus. Shape recovery usually occurs through a reversible phase transformation and, in general, has limited performance with 10% maximum strain. Here, we report the first discovery of superelastic and shape memory behavior with 12% recoverable strain in a novel intermetallic compound $CaFe_2As_2$, and discuss its unique elastic and plastic deformation behaviors in terms of a collapsed tetragonal phase transition and anisotropic stacking fault energy, respectively, with solution growth of the single crystal, in-situ micropillar compression, and density functional theory (DFT) calculations. Single crystals of $CaFe_2As_2$ were grown out from Sn flux and contains mirror-like clean facets of {0 0 1} and {3 0 1} type planes. We fabricated micropillars on these two planes, and conducted in-situ micropillar compression testing in a scanning electron microscope. The [0 0 1] $CaFe_2As_2$ micropillar exhibits unprecedented superelasticity: over 12% recoverable strain without negligible residual fatigue damage under cyclic deformation. Due to its high yield strength (2.6 GPa) and large elastic strain, it is possible to absorb and release a large amount of elastic strain energy. Also, it has potential to show one-dimensional shape memory effects at low temperatures (near 0 K) by the reversible phase transformation between the tetragonal/orthorhombic to the collapsed tetragonal phase. Furthermore, this material exhibits strong anisotropy in plasticity. For the [3 0 -1] $CaFe_2As_2$ micropillar, we found easy, preferential slip in the [1 0 0]/(0 0 1) slip system which we termed micaceous plasticity. Superelasticity and micaceous plasticity was quantitatively investigated through measuring the uni-axial stress-strain data and comparing our results to DFT calculations. DFT calculations revealed that making and breaking As-As bonds is responsible for superelasticity. A composite model was developed to monitor the volume fraction evolution of the two different phases under compression testing and successfully reproduced the experimental stress-strain curve we measured. In addition, DFT results showed a significantly low energy barrier for the [1 0 0]/(0 0 1) slip between Ca and As layers, which agrees with our experimental observation. We believe that our efforts in both experimental and computational analysis allow us to gain a fundamental understanding of the unique deformation behavior of $CaFe_2As_2$

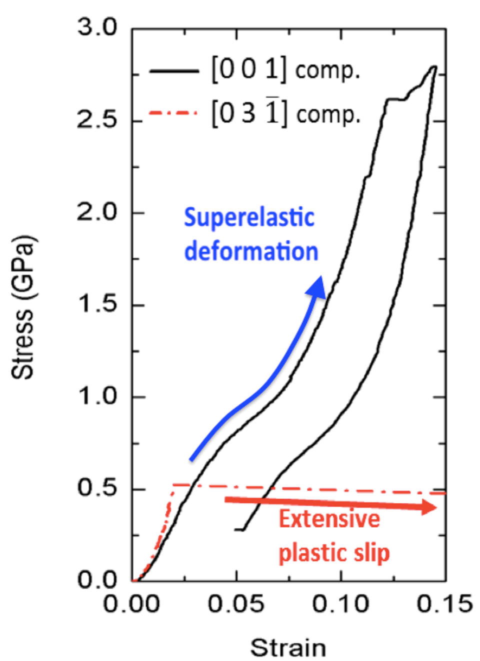

Figure 1 – A comparison of the compression stress-strain compression curves of the [0 0 1] (solid line) and [0 3 -1] directions (broken line).