Cryogenic Temperature Effects on Superelasticity of the Novel Intermetallic Compound $CaFe_2As_2$ At Small Length Scales

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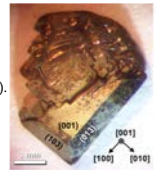
Introduction

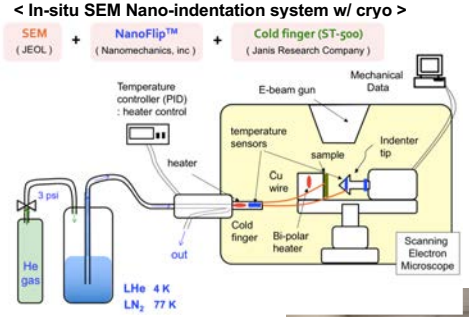
- **Materials properties of $CaFe_2As_2$ are sensitive to pressure and temperature.**
- **Reversible phase transformation** occurs from tetragonal to collapsed tetragonal phase by deformation → **Superelasticity (?)**
- The hydrostatic pressure required to induce phase transformation **decreases** as the temperature decreases. → **Temperature dependence on Superelasticity (?)**
- Solution-grown single crystals are usually too small (mm-size). Conventional bulk scale uni-axial mechanical testing is very difficult. **Small-scale** mechanical testing is necessary.
- DFT calculations can aid in understanding how the lattice collapses, the reversible solid state phase transition and their relation to superelasticity.



Methods

- **Synthesis (Ames) + Experiment (UConn) + DFT (Colorado State)**
- $CaFe_2As_2$ single crystals were solution-grown at AMES Laboratory.
- Micropillars with an aspect ratio of 2:1 having a diameter of 2μm in diameter were milled out on the single crystal using Ga+ ions in a Focused Ion Beam (FIB).
- The single crystal was then mounted in an Scanning Electron Microscope. In-situ uniaxial compression testing was performed at vacuum.
- Cryogenic testing was carried out using a custom copper cold finger with our In-situ compression system and cryogenic temperatures were reached using liquid nitrogen and liquid helium

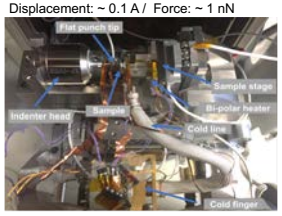
< In-situ SEM Nano-indentation system w/ cryo >

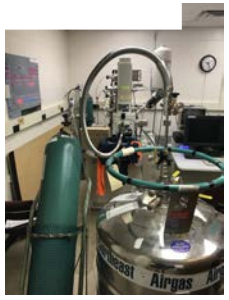


NanoFlip (Nanomechanics, inc.)

Resolutions

Displacement: ~ 0.1 A / Force: ~ 1 nN

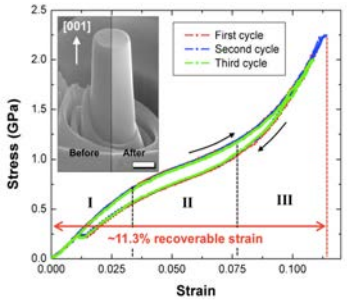




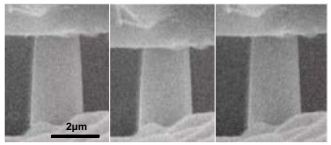
Results

1) Superelasticity of [0 0 1] $CaFe_2As_2$ under compression (300 K)

Exceptional recoverability: 3 cycles



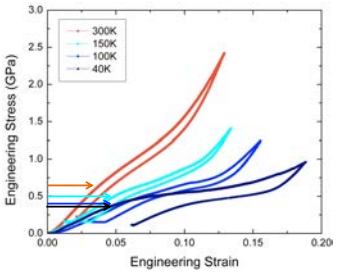
In-situ microcompression

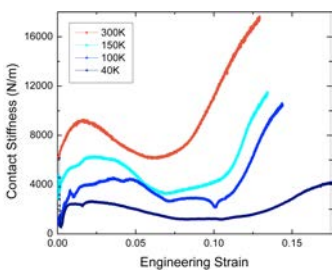


11% of deformation (Stage I, II and III) is repeatable and recoverable.

- Stage I : elastic deformation of tetragonal phase
- Stage II : **Phase transformation**
- Stage III : elastic deformation of collapsed tetragonal

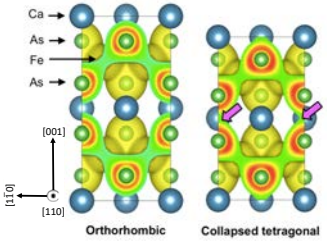
2) Cryogenic temperature testing down to 40 K





Discussion

1) Superelasticity of [0 0 1] $CaFe_2As_2$ under compression



(simulation by H. Yu and C.R. Weinberger)

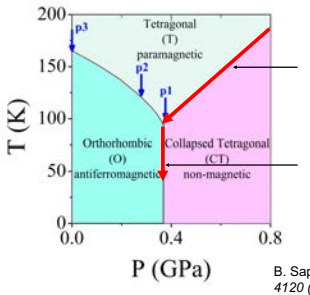
Phase transition from O (0K) to CT

The reversible phase transformation by the formation and breakage of As-As bonding

Under loading, As-As bonds form, causing the orthorhombic (tetragonal) phase to collapse, forming the collapsed tetragonal phase (See the two magenta arrows)

Unloading (under room temp.) causes the As-As bonds to break spontaneously and reverts back to the orthorhombic (tetragonal) phase

2) Decreasing on-set stress with decreasing temperature



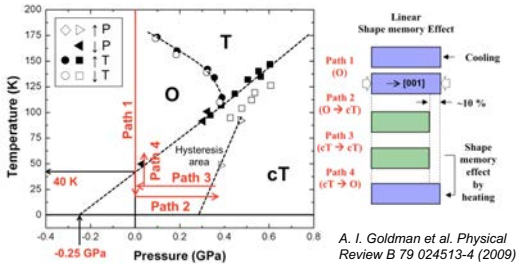
Decreasing on-set stress above 100K

Constant on-set stress below 100K

B. Saparov *et al. Sci Rep. 4, 4120 (2014).*

3) Potential linear shape memory effect at ultra-low temperatures (T < 50 K)

In-situ neutron scattering experiment under pressure



A. I. Goldman et al. Physical Review B 79 024513-4 (2009)

Concluding Remarks

- Uni-axial compression of [0 0 1] $CaFe_2As_2$ micropillar exhibits super-elasticity up to ~ 13.4 maximum recoverable strain.
- The reversible phase transition between tetragonal and collapsed tetragonal phases produces the large recoverable strain **(SUPERELASTICITY)**.
- The reversible phase transformation even occurs under temperatures down to 39 K, however, the on-set stress of phase transformation decreases as temperature decreases down to 100 K.
- There is promising potential for linear shape memory effect at low temperatures (T < 50K)

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