THE UNIVERSITY of TENNESSEE UT KNOXVILLE

Experimental and Computational Investigation of High-Entropy Alloys (HEAs) for Elevated Temperature Applications

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- **Ph.D. Students: Haoyan Diao[1], Zhi Tang[1], and Louis J. Santodonato[1]**
- **Research Associates: Gongyao Wang[1] and Xie Xie[1]**
- **Collaborators: Chuan Zhang[2], K. A. Dahmen[3], and Shizhong Yang[4]**

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4. Southern University and A&M College, Baton Rouge LA 70807

CompuTherm FOR MATERIALS DESIGN

ILLINOIS UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

Acknowledgements

We are very grateful to:

- Vito Cedro
- Richard Dunst
- Patricia Rawls
- Jessica Mullen
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- Steven Markovich
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Outline of Presentation

- Background and Unique Features of HEAs
- Microstructural Characterization
- Mechanical Behavior
- Published Papers and Presentations
- Conclusions
- Future Work

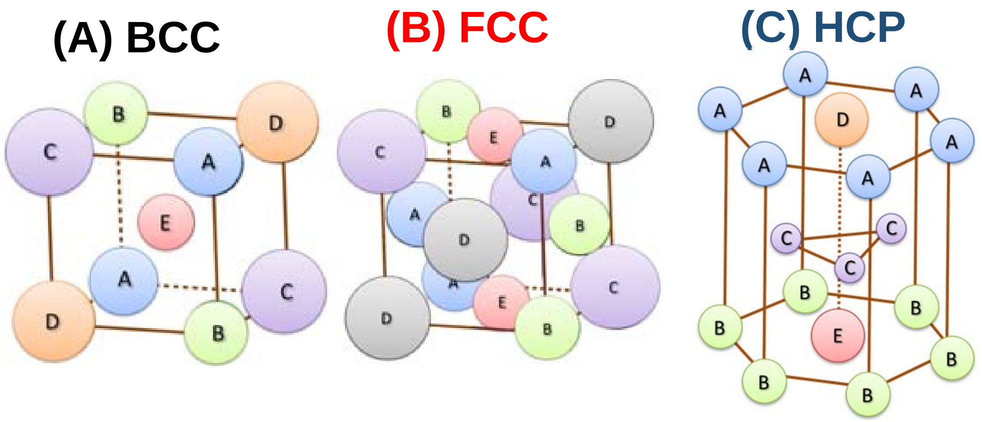
Background and Unique Features

- Most alloy systems are based on a single principal element to form the matrix.
- Important characteristics of high-entropy alloys (HEAs):

✓ **An identity crisis – 5 or more elements (no single element) dominates [5 atomic percent (at.%) - 35 at.%]**

✓ **Relatively-high configurational entropy (influences stability)**

✓ **Relatively-large lattice strains (influences strength and stability)**


(A) BCC (B) FCC (C) HCP

BCC: Body-Centered Cubic; FCC: Face-Centered Cubic; HCP: Hexagonal close packed

1. J. W. Yeh, S. K. Chen, S. J. Lin, J. Y. Gan, T. S. Chin, T. T. Shun, C. H. Tsau, and S. Y. Chang, Advanced Engineering Materials 6, 299 (2004).
2. B. Cantor, I. T. H. Chang, P. Knight, and A. J. B. Vincent, Materials Science and Engineering A 375-377, 213 (2004).
3. Y. Zhang, T. T. Zuo, Z. Tang, M. C. Gao, K. A. Dahmen, P. K. Liaw, and Z. P. Lu, Progress in Materials Science 61, 1 (2014).
4. L. J. Santodonato, Y. Zhang, M. Feygenson, C. M. Parish, M. C. Gao, R. J. Weber, J. C. Neuefeind, Z. Tang, and P. K. Liaw, Nature Communications 6, 5964 (2015).
5. Takeuchi, K. Amiya, T. Wada, K. Yubuta, and W. Zhang. JOM, 66, 10 (2014).
6. K. M. Youssef, A. J. Zaddach, C. Niu, D. L. Irving, and C. C. Koch. Materials Research Letters, 1-5 (2014).
7. M. C. Gao and D. E. Alman, Entropy 15(10), 4504-4519 (2013).
8. M. Feuerbacher, M. Heidelmann, and C. Thomas, Materials Research Letters 3(1), 1-6 (2014).

Background and Unique Features (Cont'd)

- In equimolar ratios,

$$\Delta S_{conf} = k_B \cdot \ln(\Omega) = \frac{R}{N_A} \ln(N)^{N_A} = R \cdot \ln(N)$$

k: Boltzmann's constant

Ω: Number of ways of mixing

R: Gas Constant

N: Number of elements

N_A: Avogadro constant

High entropy of mixing and sluggish diffusion yield stable FCC, BCC, or HCP solid solutions.

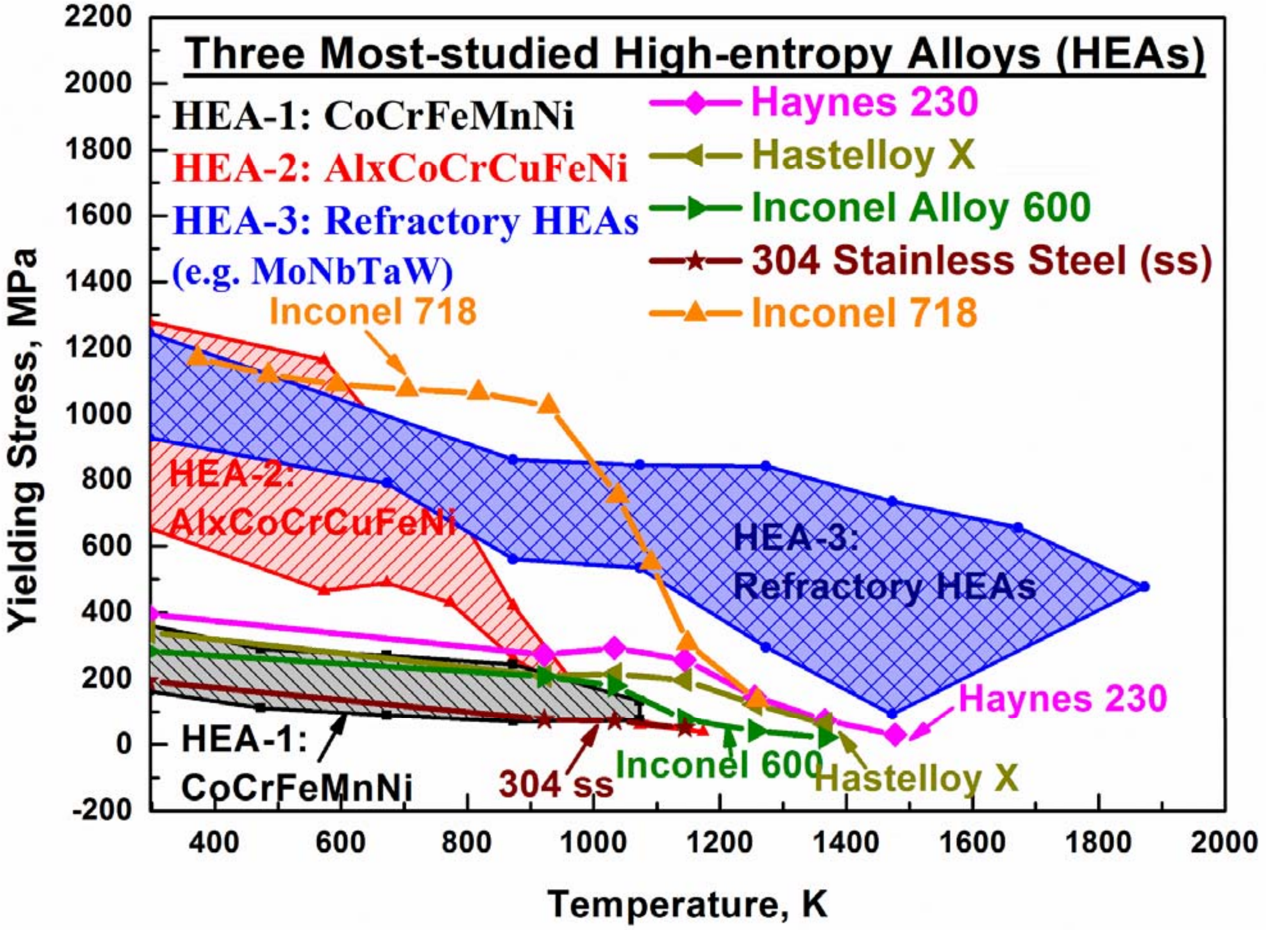
- Stable phases have the lowest Gibbs Free Energy

$$\Delta G = \Delta H - T\Delta S$$

G: Gibbs free energy
H: Enthalpy
T: Temperature
S: Entropy

At high temperatures, HEAs are stable and show great high-temperature strengths.

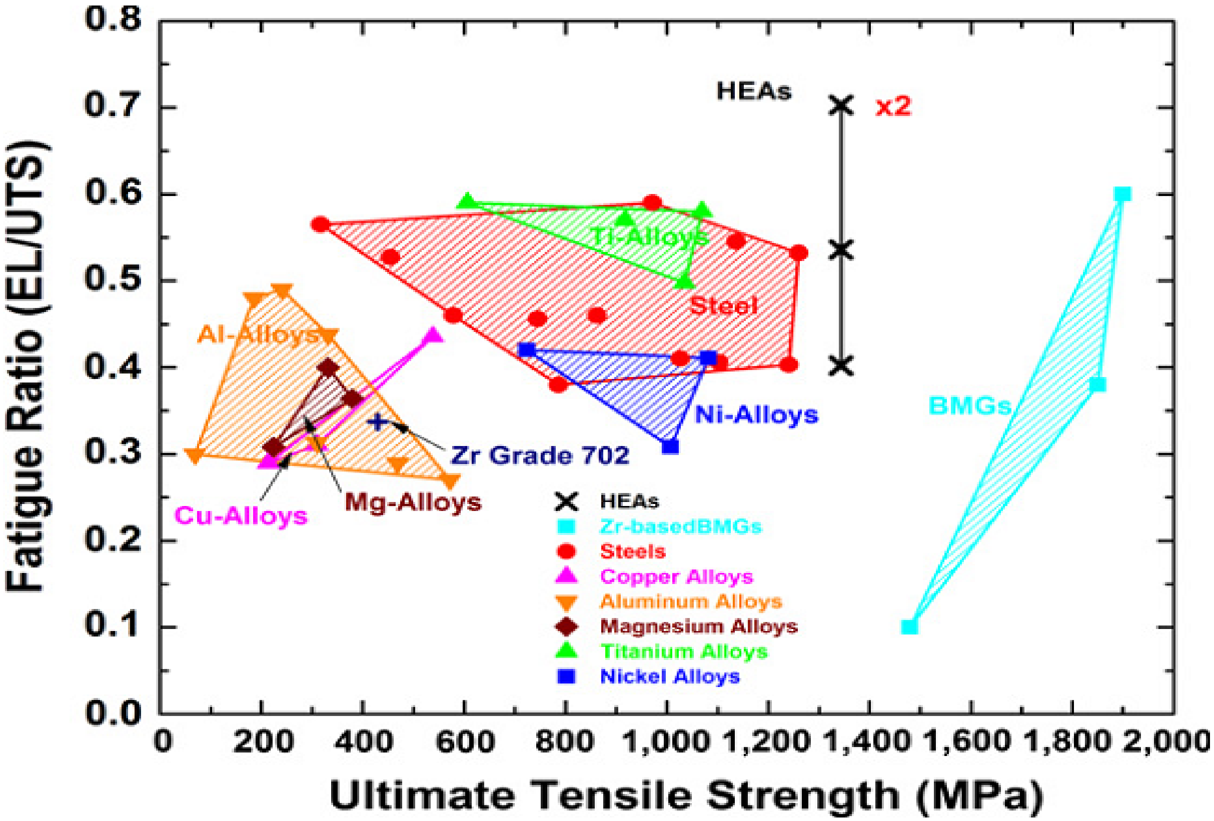
Background and Unique Features (Cont'd)



H. Diao, X. Xie, R. Feng, B. Chen, C. Zhang, F. Zhang, K. A. Dahmen, and P. K. Liaw, "Mechanical Behavior of Single-phase High-entropy Alloys (HEAs): An overview", in preparation.

Background and Unique Features (Cont'd)

Good Fatigue Resistance of Al0.5CoCrCuFeNi

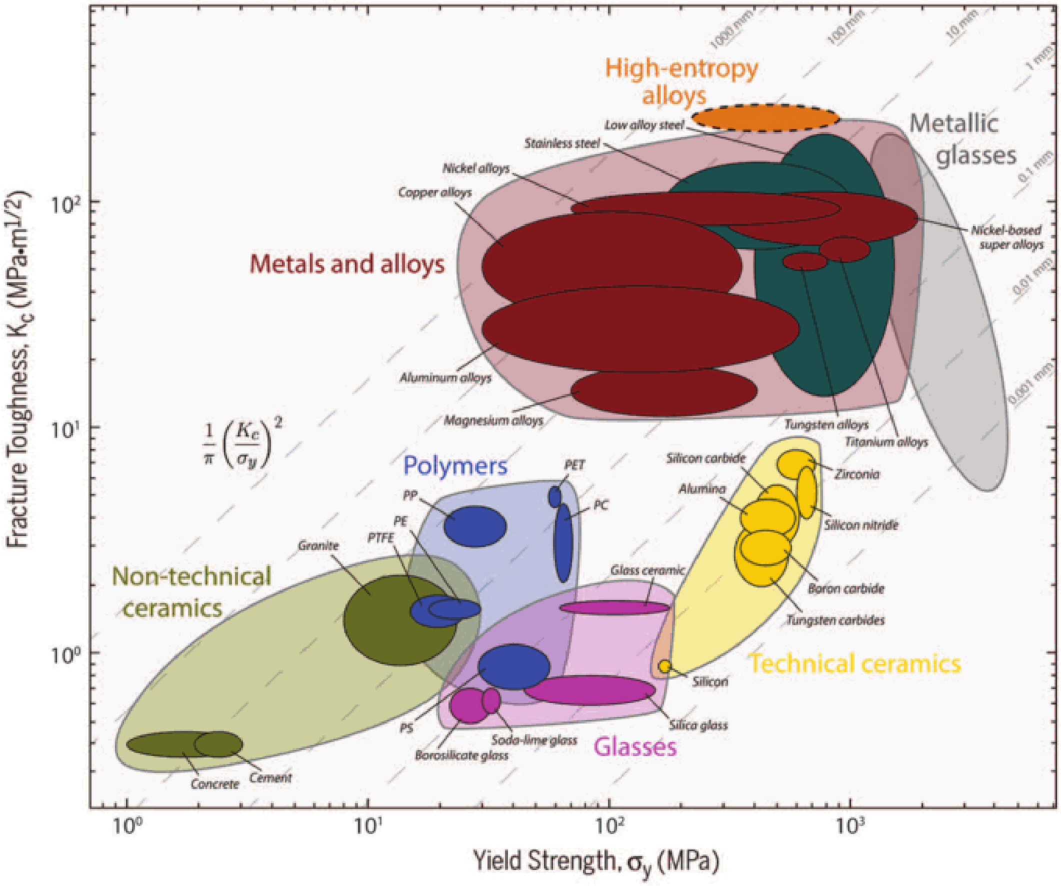


EL: Fatigue-Endurance Limit   UTS: Ultimate Tensile Strength

M. A. Hemphill, T. Yuan, G. Y. Wang, J. W. Yeh, C. W. Tsai, A. Chuang, and P. K. Liaw, Acta Materialia 60, 5723 (2012).

Background and Unique Features (Cont’d)

Good Fracture Toughness at 77 K of CoCrFeMnNi



B. Gludovatz, A. Hohenwarter, D. Catoor, E. H. Chang, E. P. George, and R. O. Ritchie, *Science*, 2014, 345(6201), pp. 1153-8.

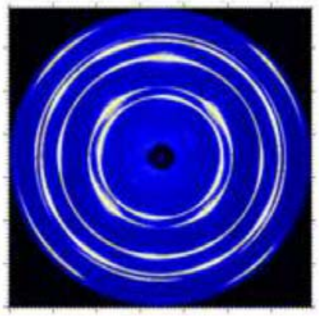
Objectives

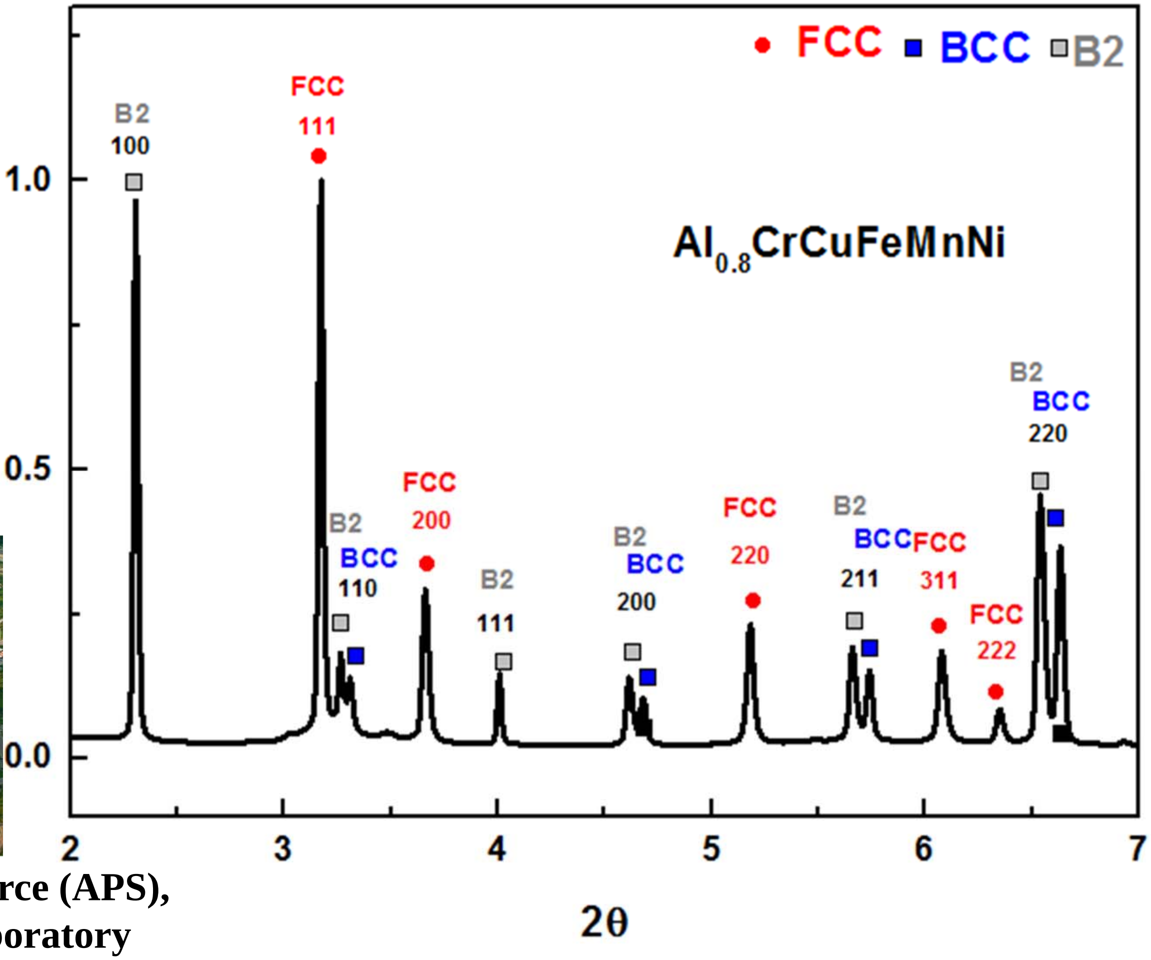
- Provide a fundamental study of a new HEA system, AlxCrCuFeMnNi (x = 0.1 and 0.8), which is based on AlxCrCuFeCoNi (HEA-2), since Mn is less expensive than Co
  - To investigate microstructural characteristics, using synchrotron X-ray diffraction and thermodynamic modeling
  - To obtain mechanical properties, using compression tests
  - To examine the thermal stability at high temperatures, employing synchrotron and neutron diffraction
  - To perform nanoindentation creep studies at room temperature
- Conduct a scientific investigation of a single-phase $Al_{0.3}$CoCrFeNi
  - To study microstructure evolution
  - To develop hardness, compression, and in-situ tension properties
  - To investigate conventional creep behavior

Microstructural Characterization

❑Aluminum-ratio effects

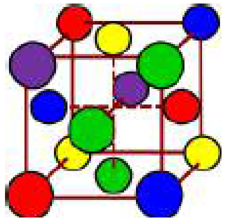
Synchrotron X-ray Diffraction Pattern





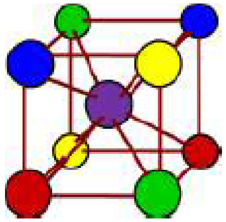
Advanced Photon Source (APS),
Argonne National Laboratory

Face-centered Cubic (FCC)



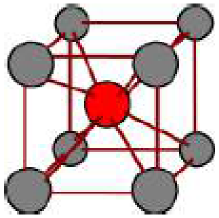
0.3692 nm

Body-centered Cubic (BCC)



0.2888 nm

B2 structure

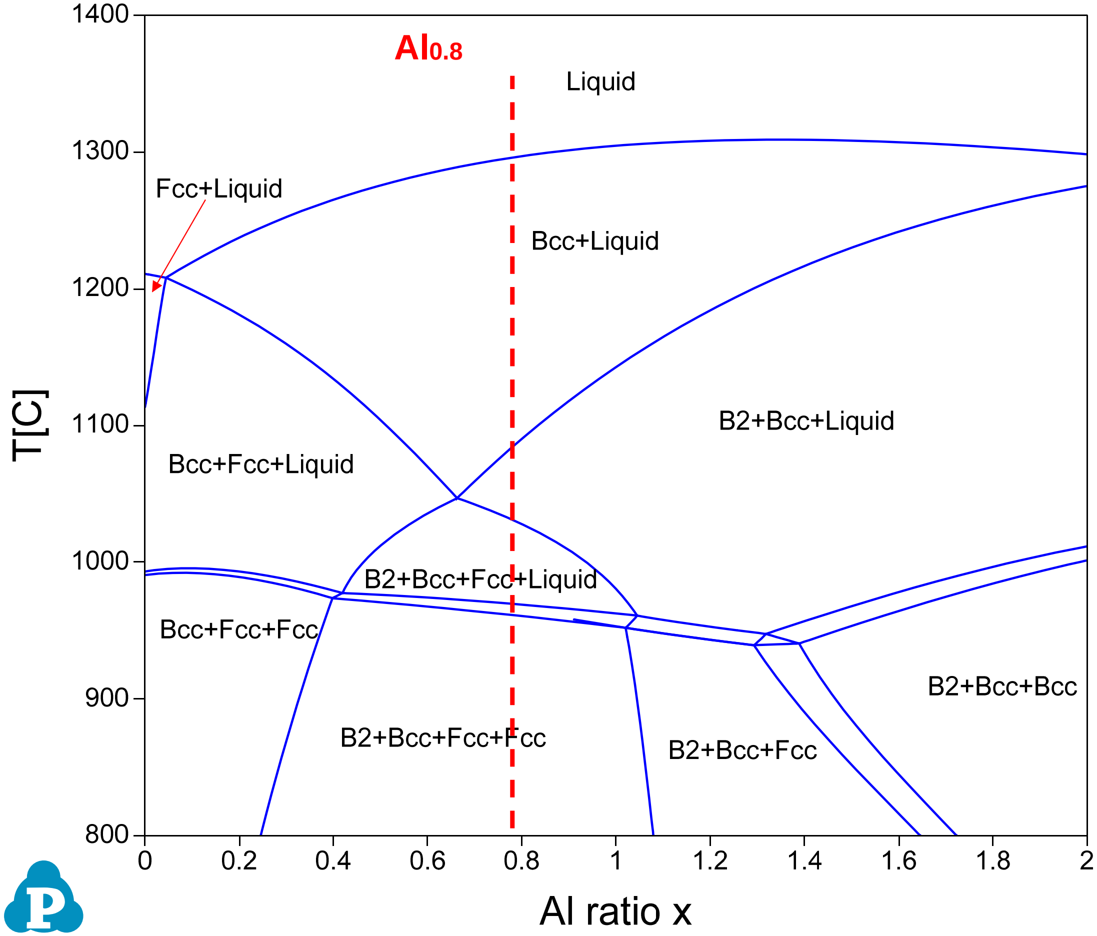


0.2928 nm

Microstructural Characterization (Cont'd)

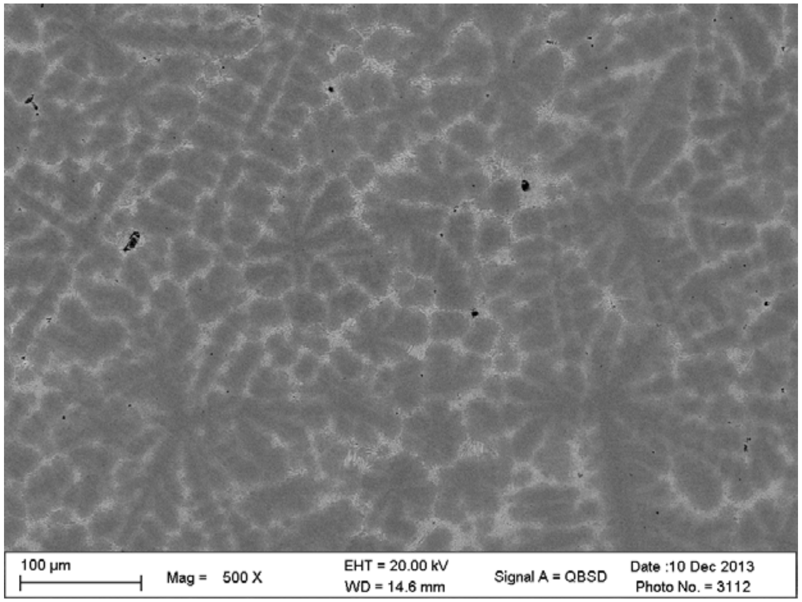
❑Aluminum-ratio effect

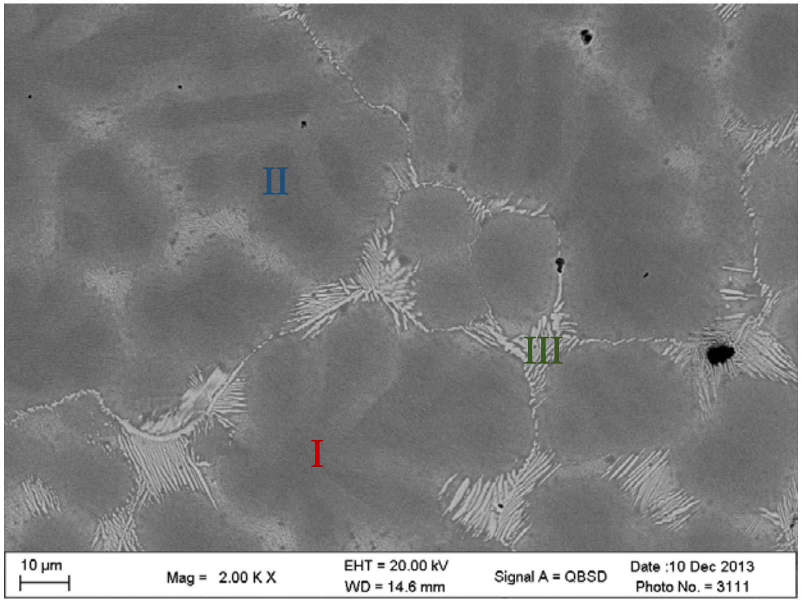
Thermodynamic Modeling



Microstructures - Al0.8CrCuFeMnNi

❑Phase-segregation behavior

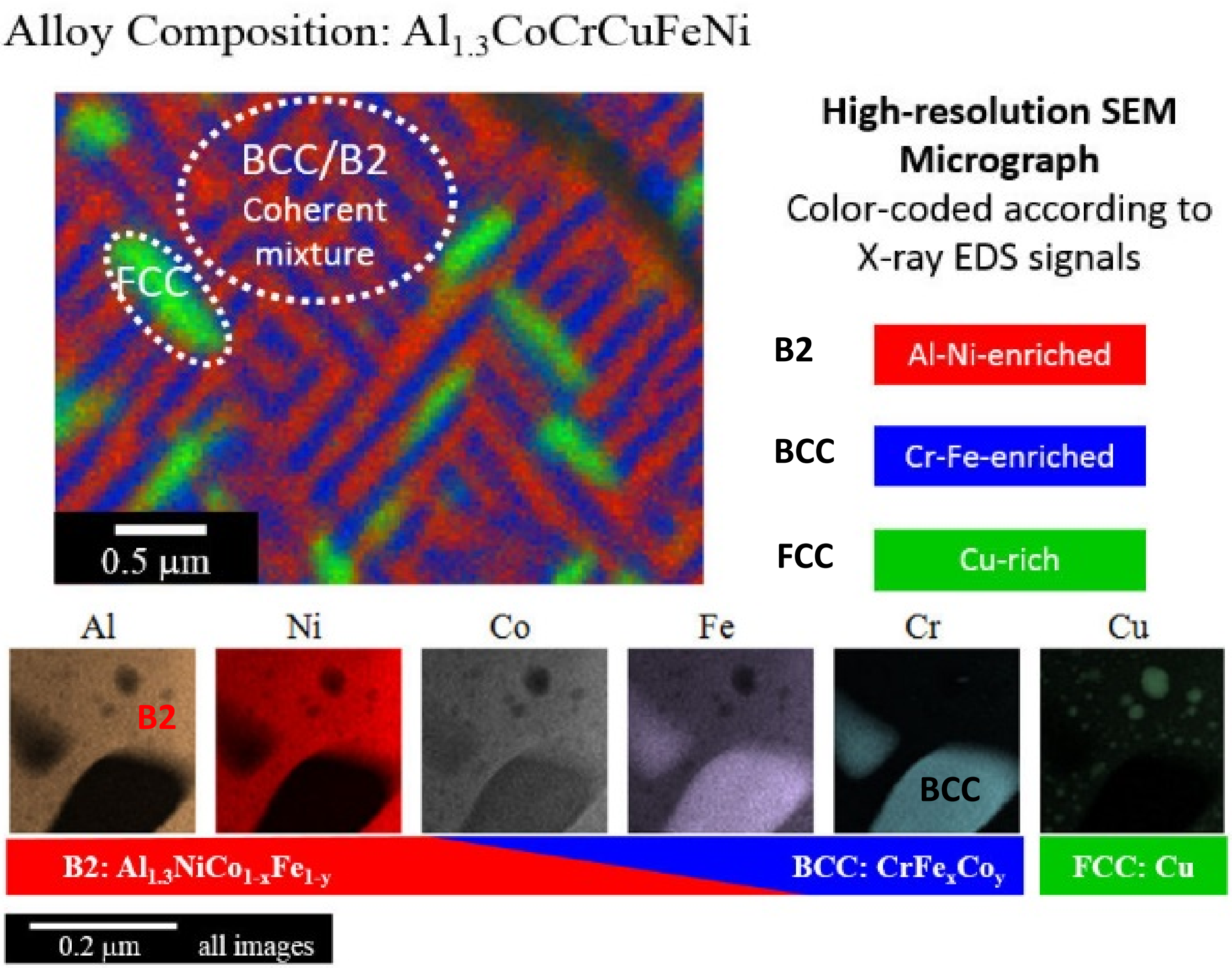




Atomic %	**Al**	**Cr**	**Mn**	**Fe**	**Ni**	**Cu**
Nominal	13.79	17.24	17.24	17.24	17.24	17.24
Light-grey area (I)	20.97	4.86	19.31	6.59	28.13	20.14
Dark-grey area (II)	8.12	31.88	15.47	29.04	9.05	6.44
White-phase layer (III)	6.97	1.65	19.12	3.11	9.90	59.25

Microstructures – Al1.3CoCrCuFeNi

❑Phase-segregation behavior



At room temperature (RT)

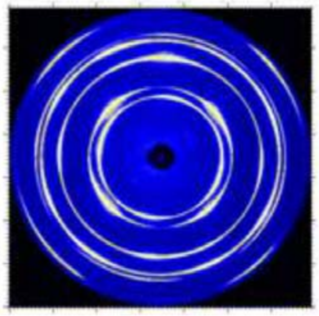
Scanning electron microscopy (SEM)

Energy-dispersive spectroscopy (EDS)

L. J. Santodonato, Y. Zhang, M. Feygenson, C. M. Parish, M. C. Gao, R. J. Weber, J. C. Neuefeind, Z. Tang, and P. K. Liaw, *Nature Communications*, 2015, 6, pp. 5964.

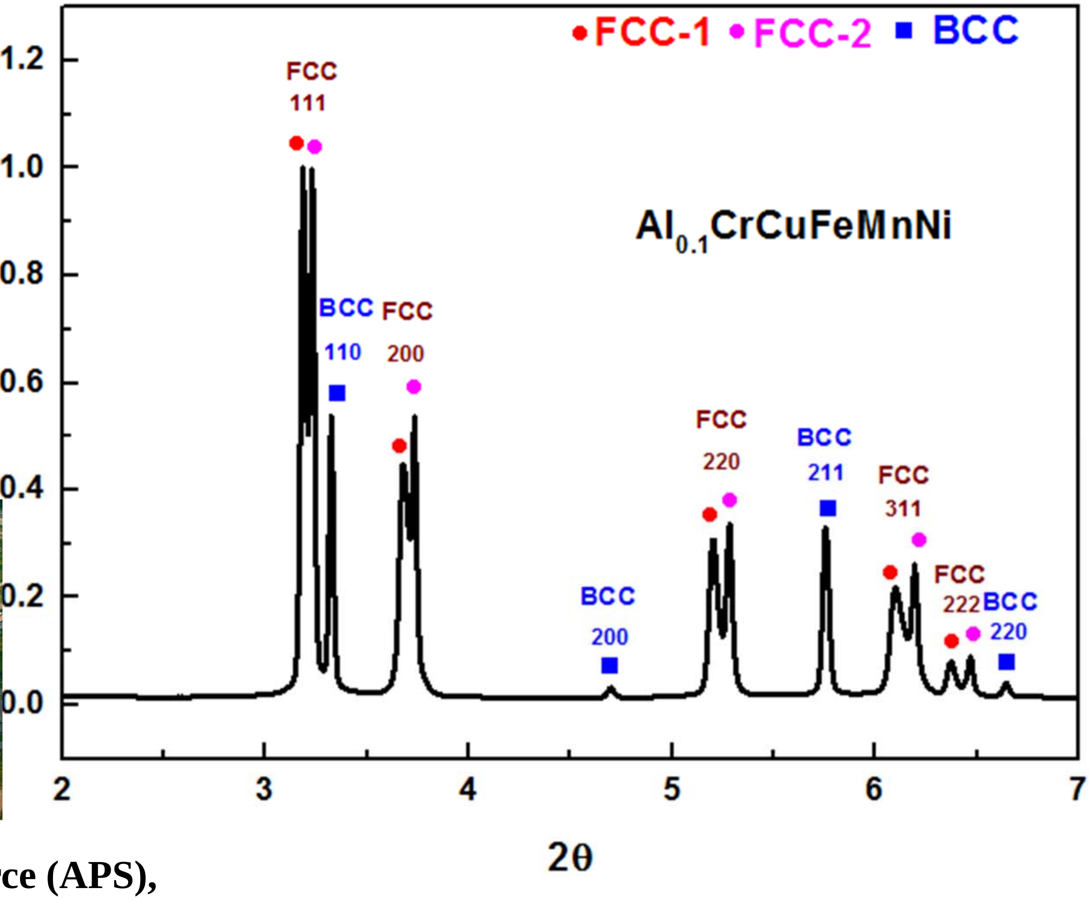
Microstructural Characterization

❑Aluminum-ratio effects

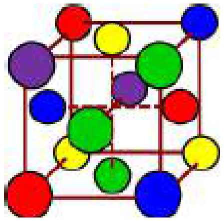


Advanced Photon Source (APS), Argonne National Laboratory

Synchrotron X-ray Diffraction Pattern

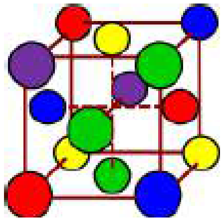


Face-centered Cubic (FCC-1)



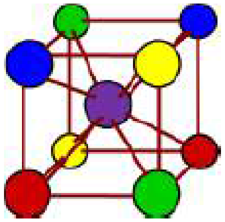
0.3677 nm

Face-centered Cubic (FCC-2)



0.3622 nm

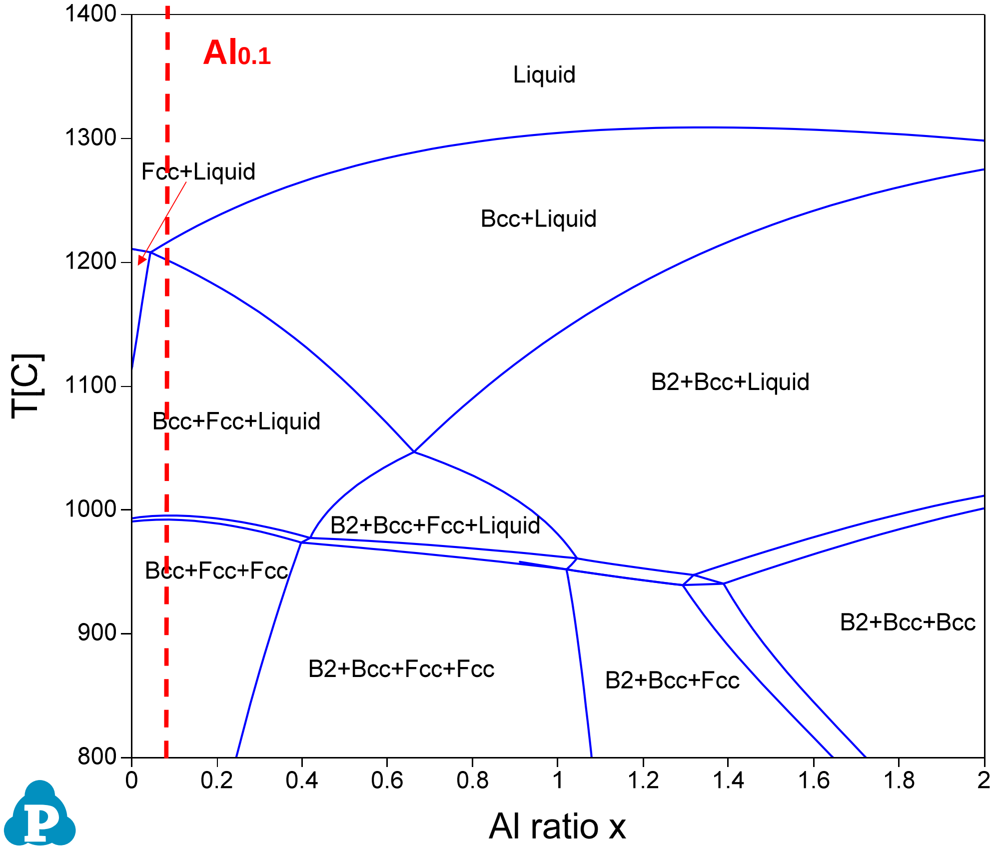
Body-centered Cubic (BCC)



0.2888 nm

Microstructural Characterization (Cont’d)

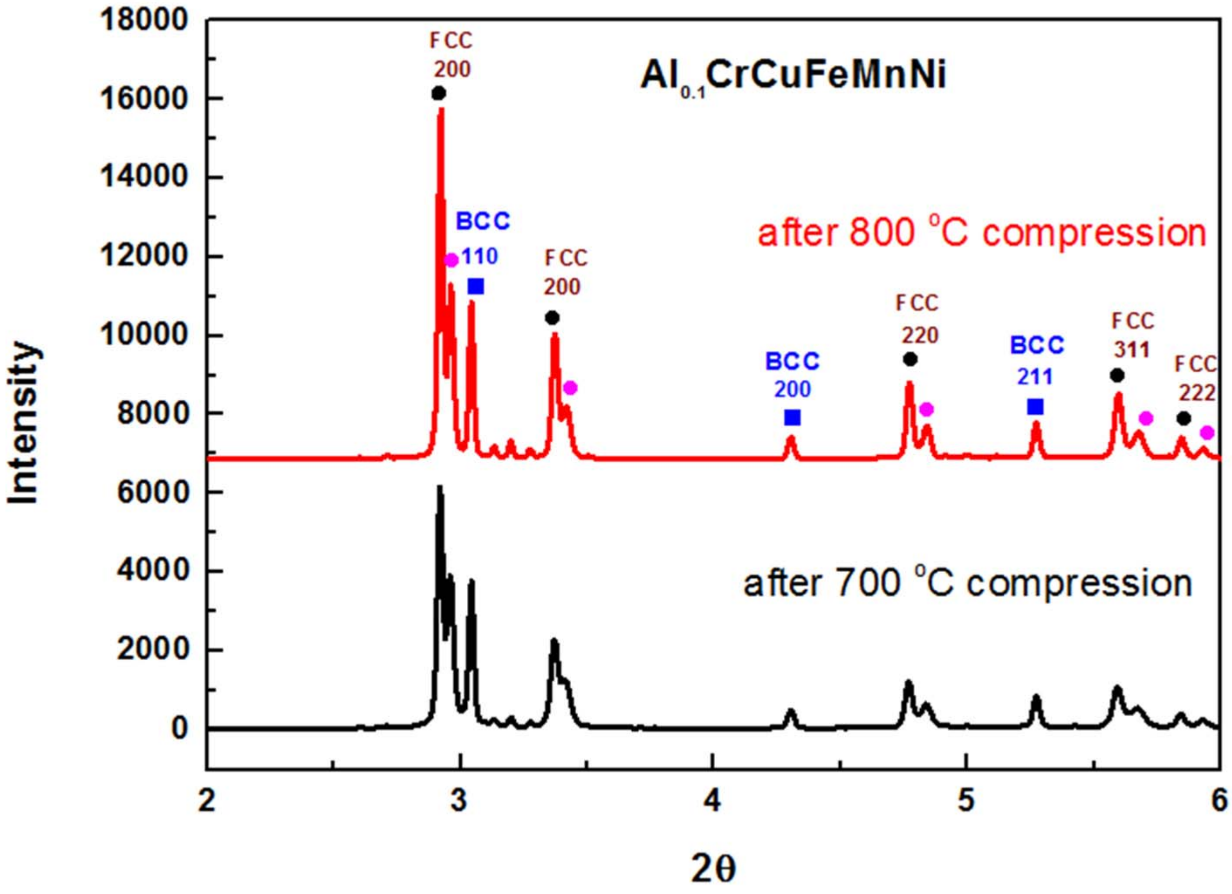
- **Aluminum-ratio effect**

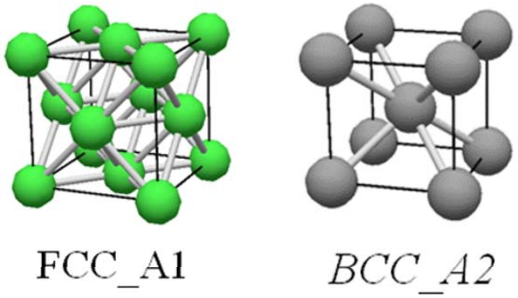


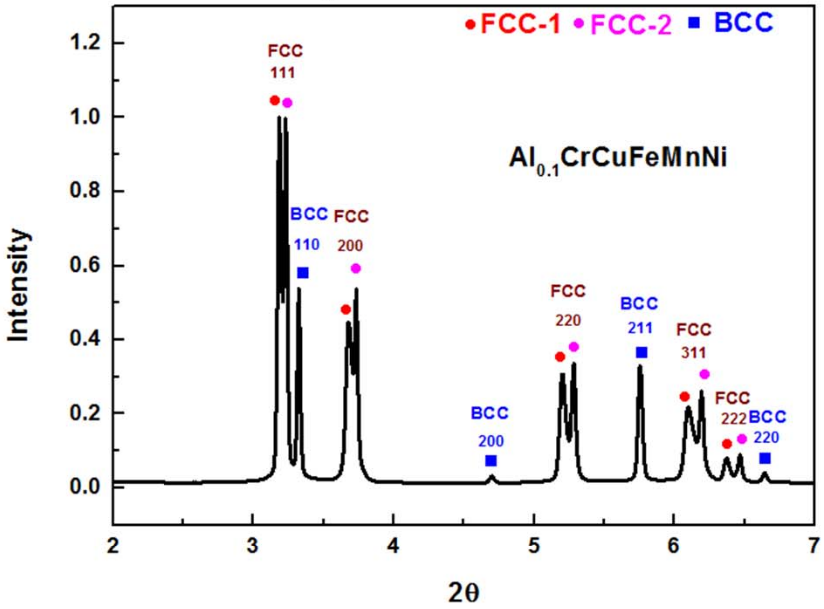
Thermodynamic Modeling

Synchrotron X-ray Diffractions after Hot Compression

- ❑**Thermal stability**

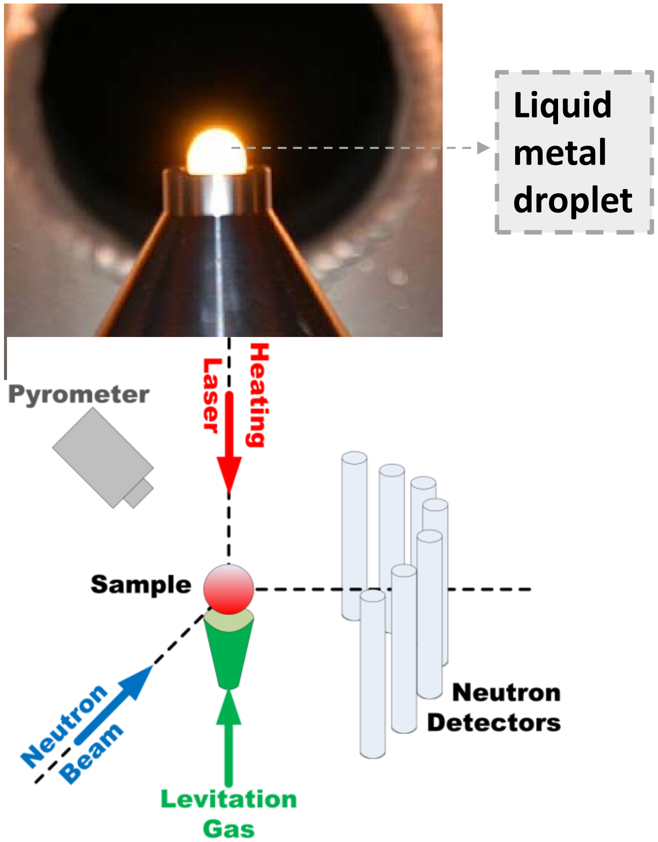






In-situ Neutron Levitation Results

Spallation Neutron Source (SNS), Oak Ridge National Laboratory (ORNL)



The Nanoscale-Ordered Materials Diffractometer (NOMAD)

L. J. Santodonato, Y. Zhang, M. Feygenson, C. M. Parish, M. C. Gao, R. J. Weber, J. C. Neuefeind, Z. Tang, and P. K. Liaw, *Nature Communications*, 2015, 6, pp. 5964.

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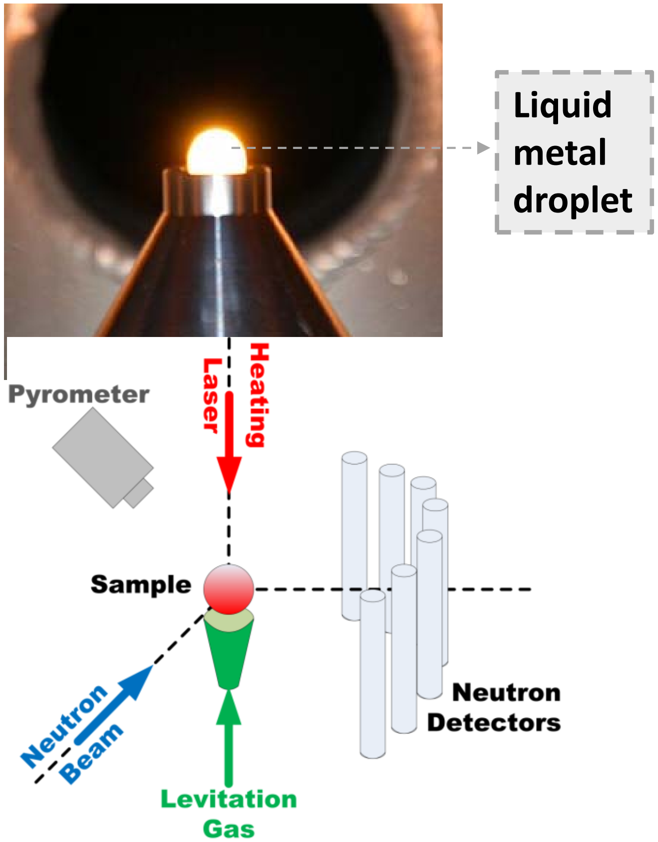
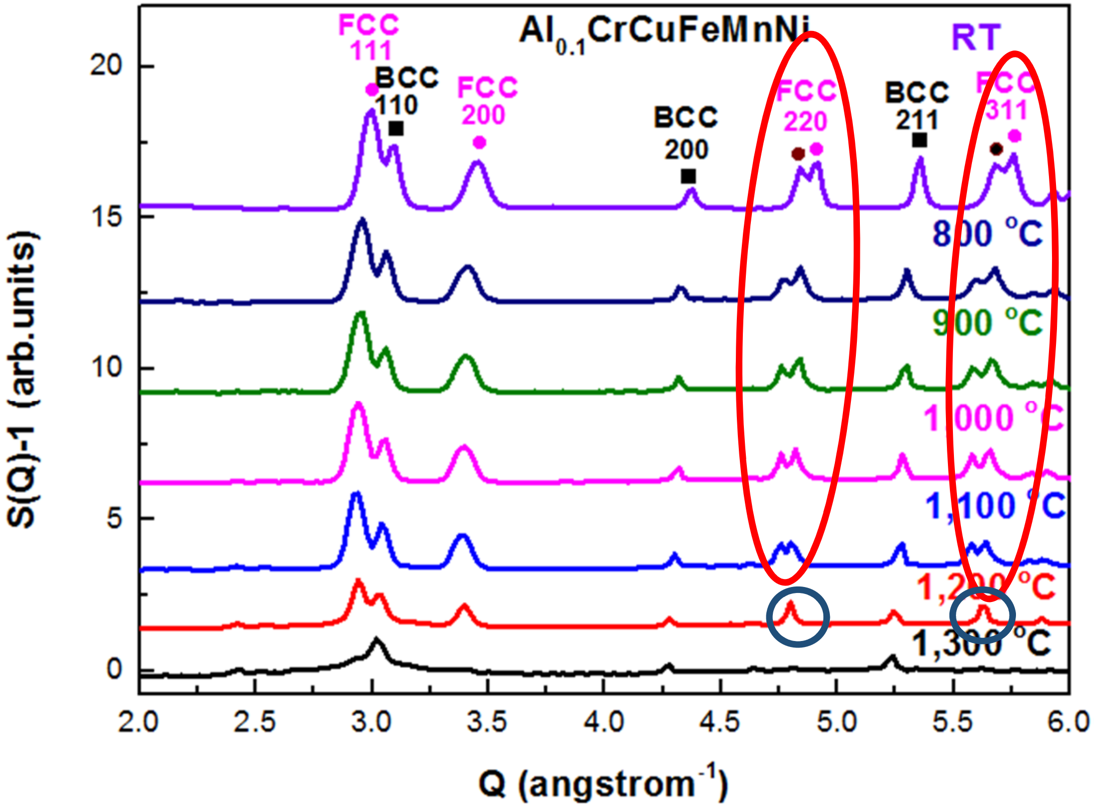
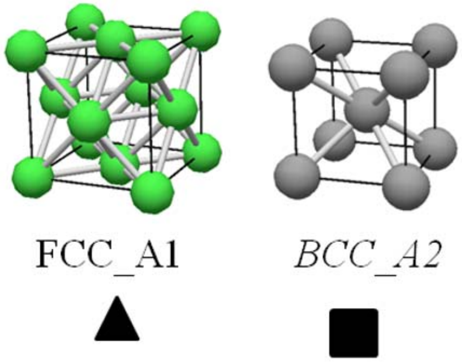


L. J. Santodonato, Y. Zhang, M. Feygenson, C. M. Parish, M. C. Gao, R. J. Weber, J. C. Neuefeind, Z. Tang, and P. K. Liaw, *Nature Communications*, 2015, 6, pp. 5964.

In-situ Neutron Levitation Results



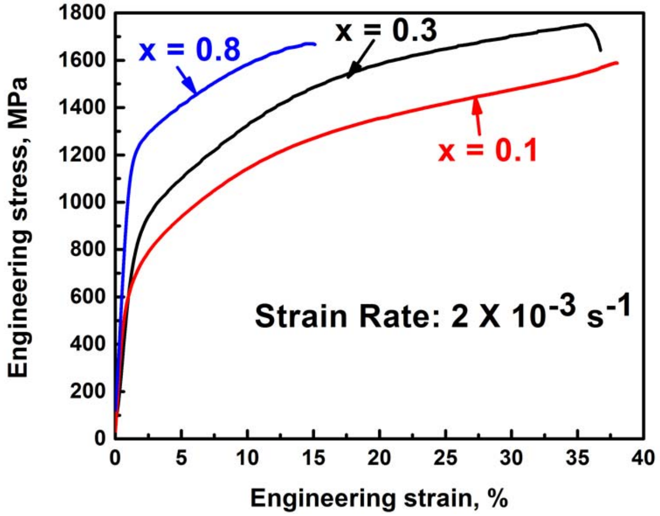


❑In the range of RT to 1,100 °C
FCC 1 + FCC 2 + BCC

❑1,200 °C
FCC 1 + BCC

❑1,300 °C
BCC

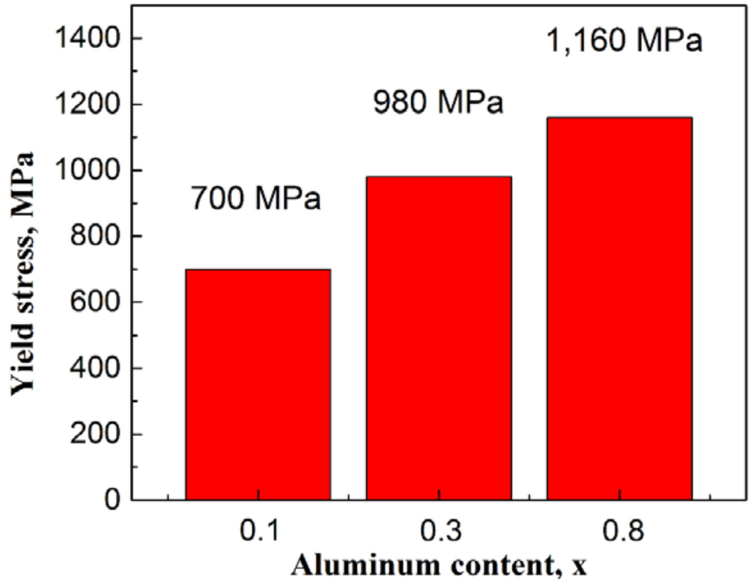
Compression Tests (Aluminum-ratio Effect)

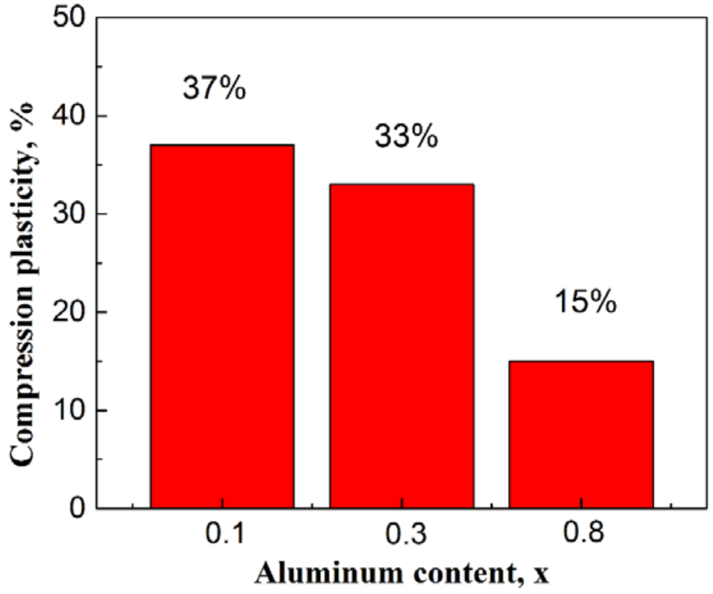


As the aluminum content increases,

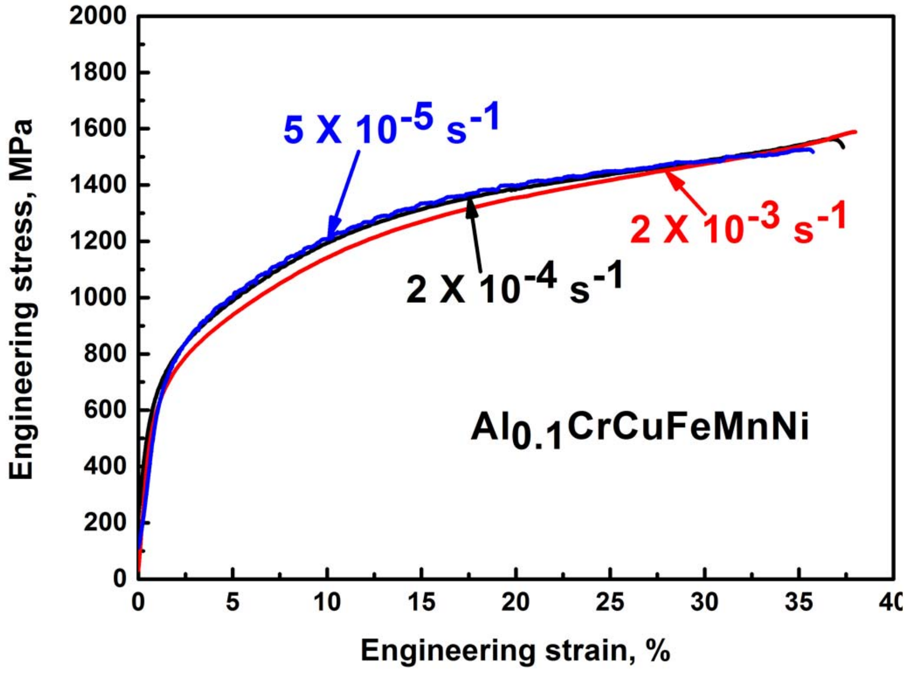
- **Yield stress increases**
- **Compression plasticity decreases**

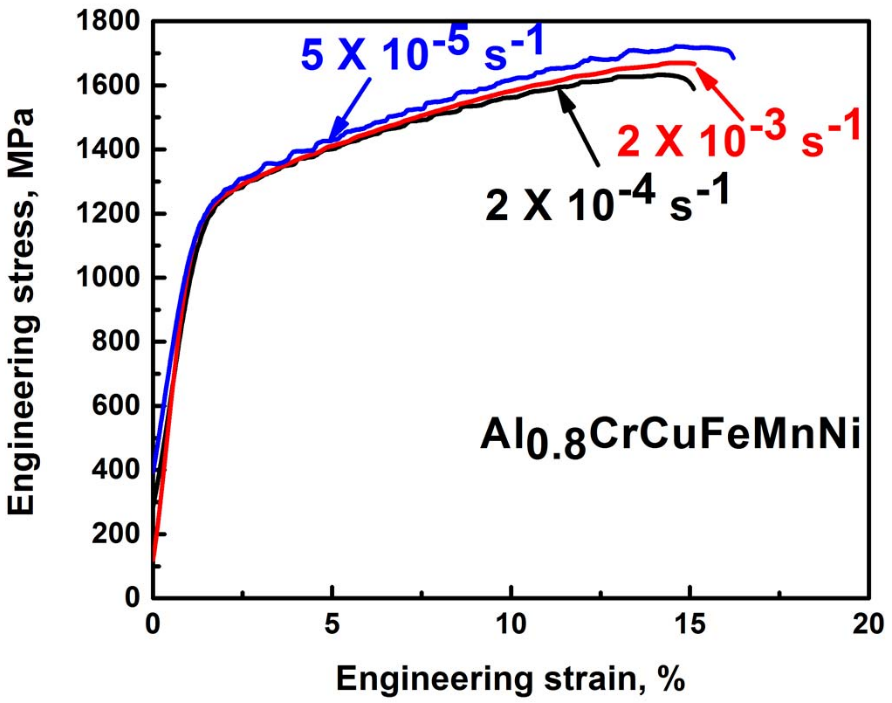
This phenomenon is due to the increased strengthening effect of lattice strains caused by the lattice-sites occupation of Al.





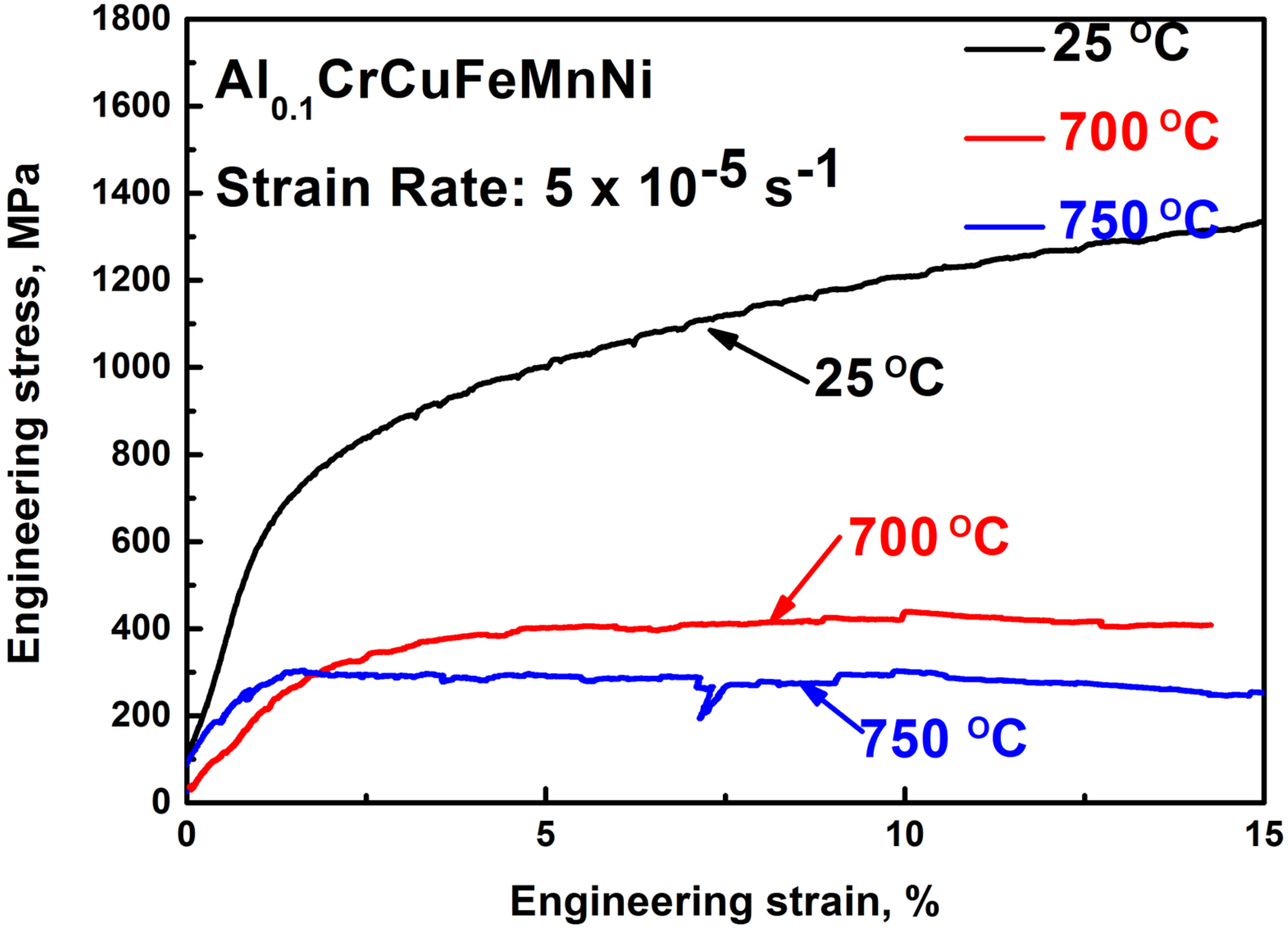
Compression Tests (Strain-rate Effect)



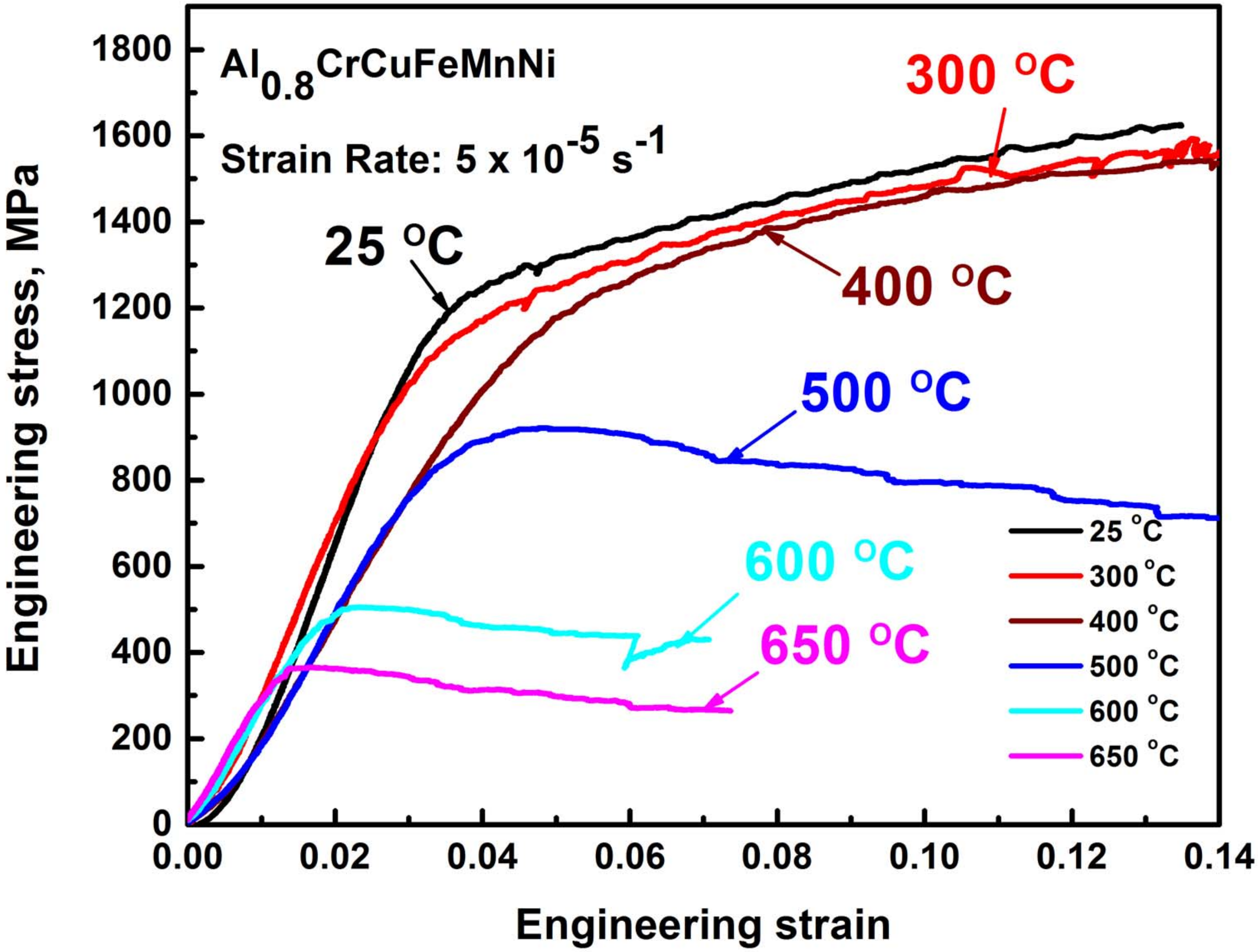


The mechanical properties at room temperature are insensitive to strain rates

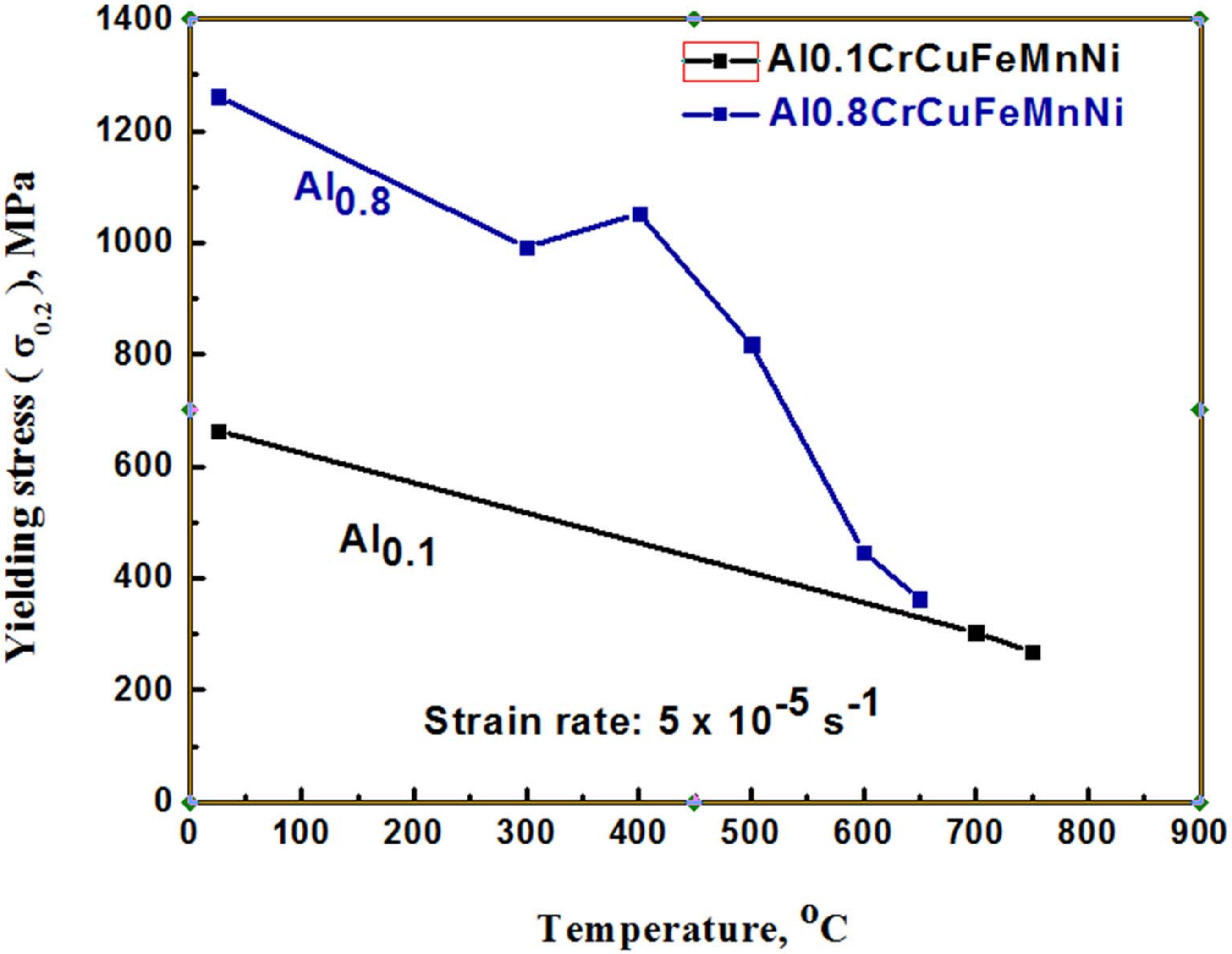
Compression Tests (Temperature Effect)



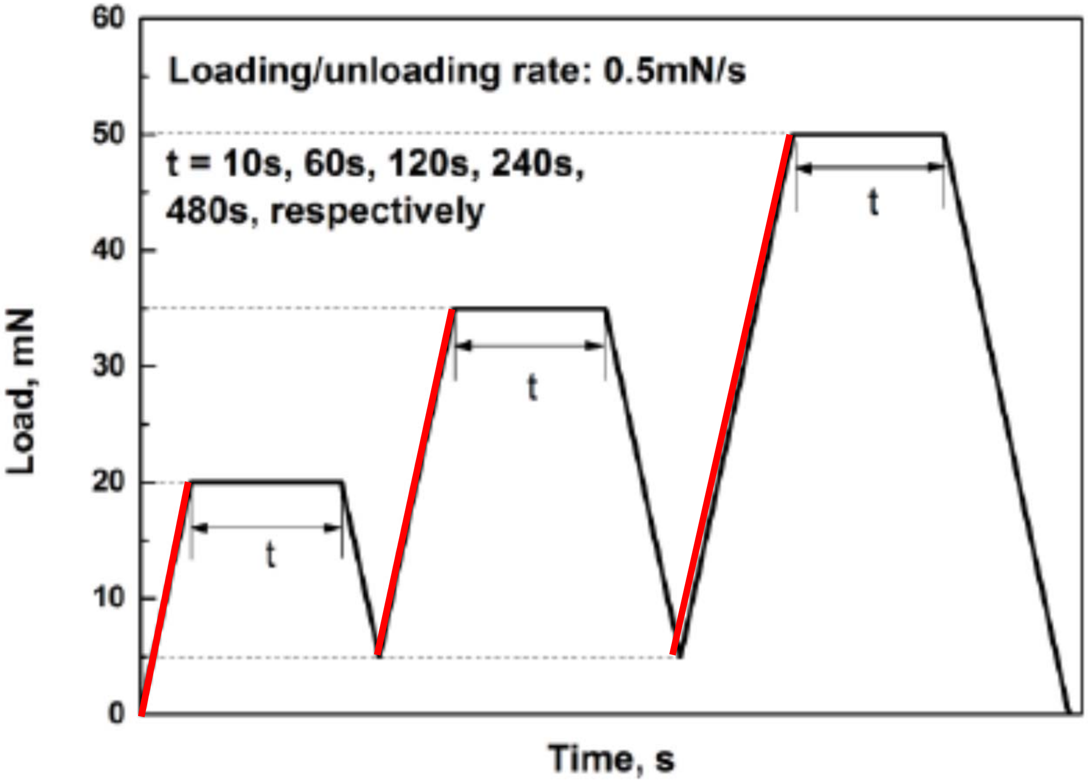
Compression Tests (Temperature Effect, Cont'd)



Compression Tests (Temperature Effect, Cont'd)



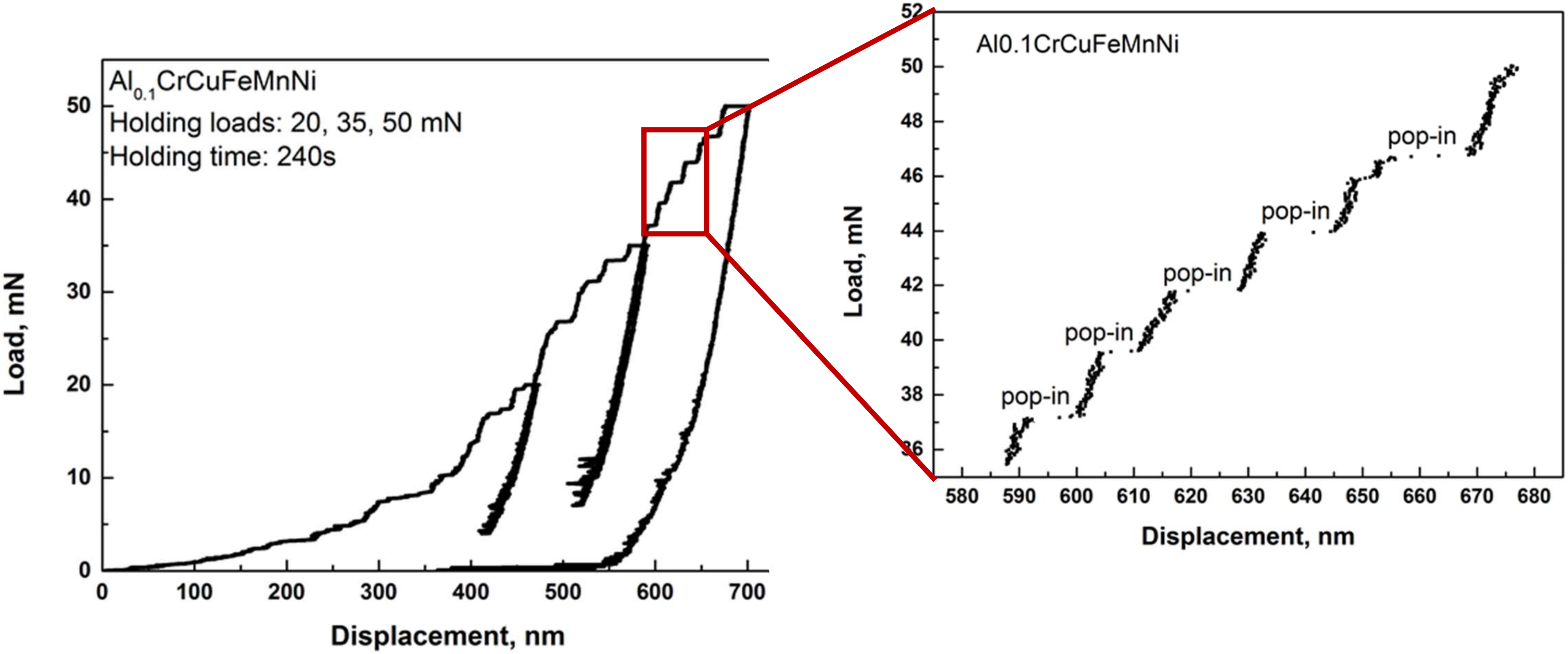
Nanoindentation Creep



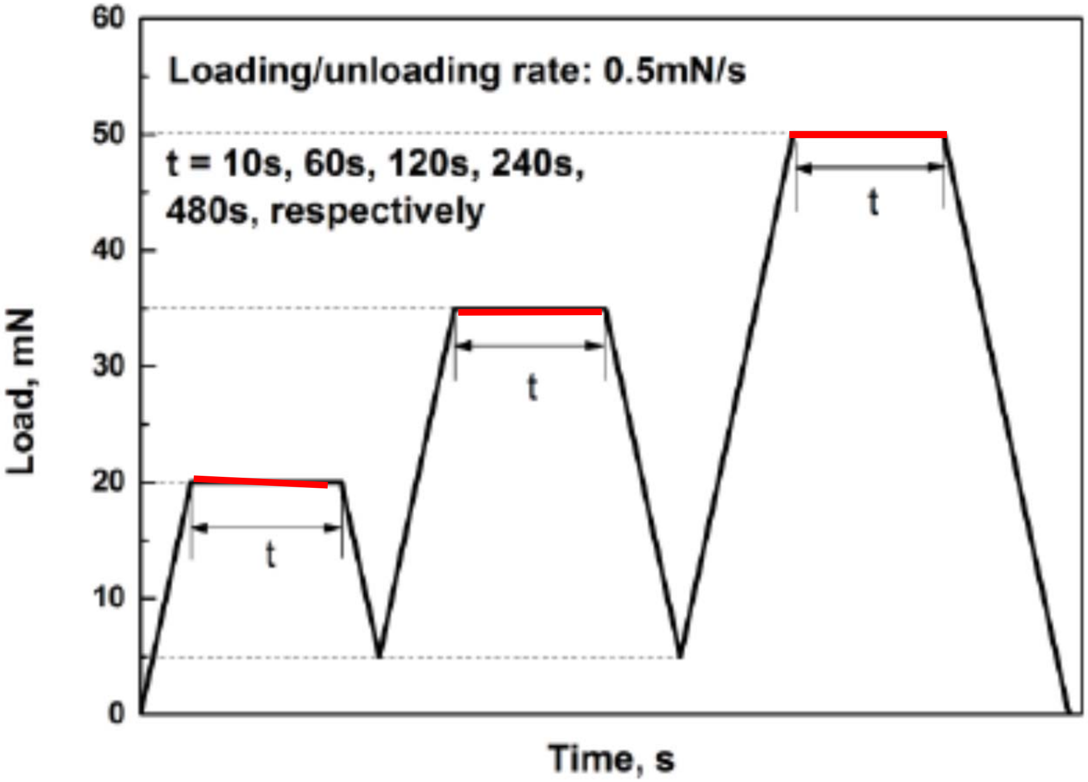
- Each test consists of 3 loading-unloading cycles
- The loading segment reaches the preset peak load of 20, 35, and 50 mN at a loading rate of 0.5 mN/s. Unloaded at the same loading rate
- The load is kept for 10 s, 60 s, 240 s, and 480 s

Nanoindentation Creep (Cont'd)

Loading-unloading load-displacement curves



Nanoindentation Creep (Cont'd)



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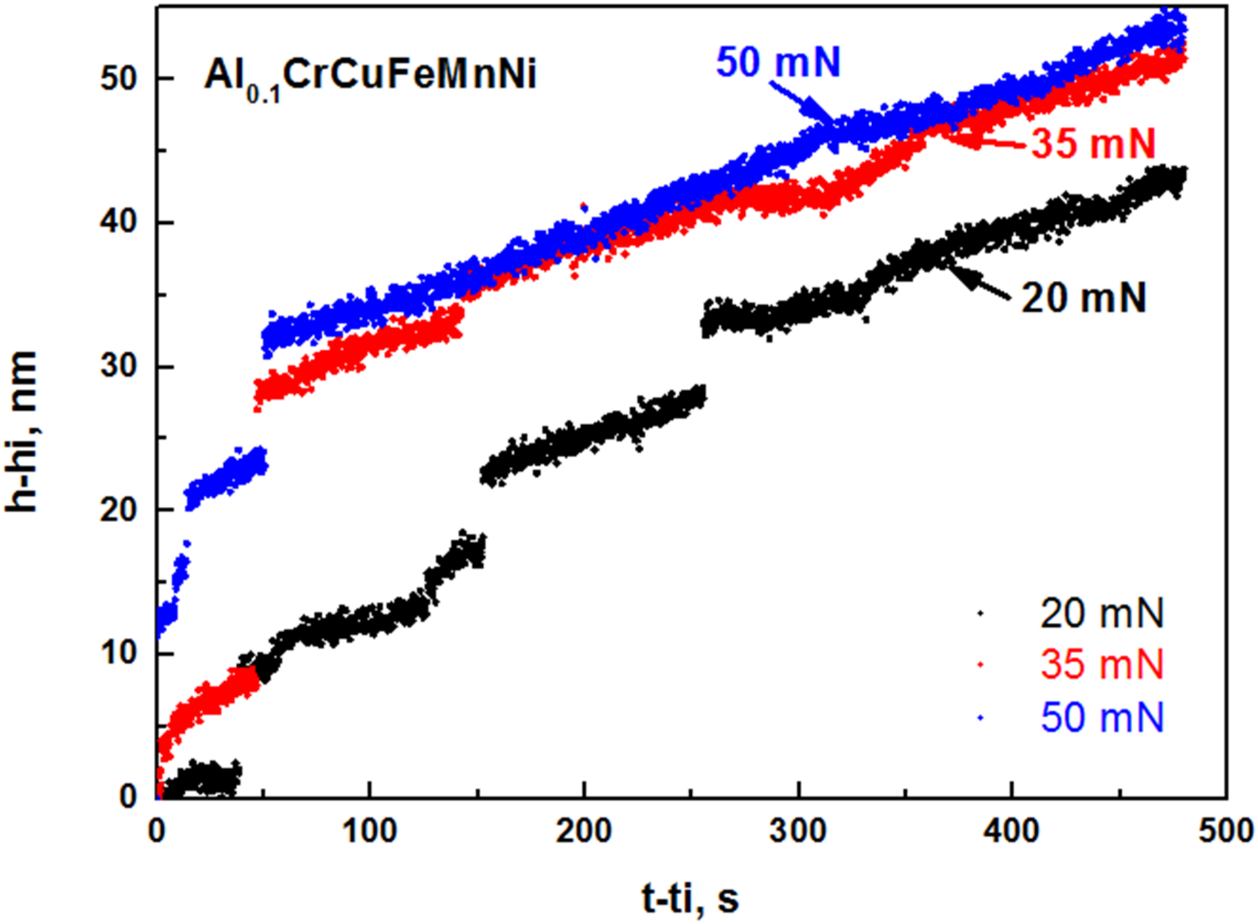
- The load is kept for 10, 60, 240, and 480 s

Nanoindentation Creep (Cont'd)

At a constant load, serrations happen.



Nanoindentation Creep (Cont'd)

Empirical equation

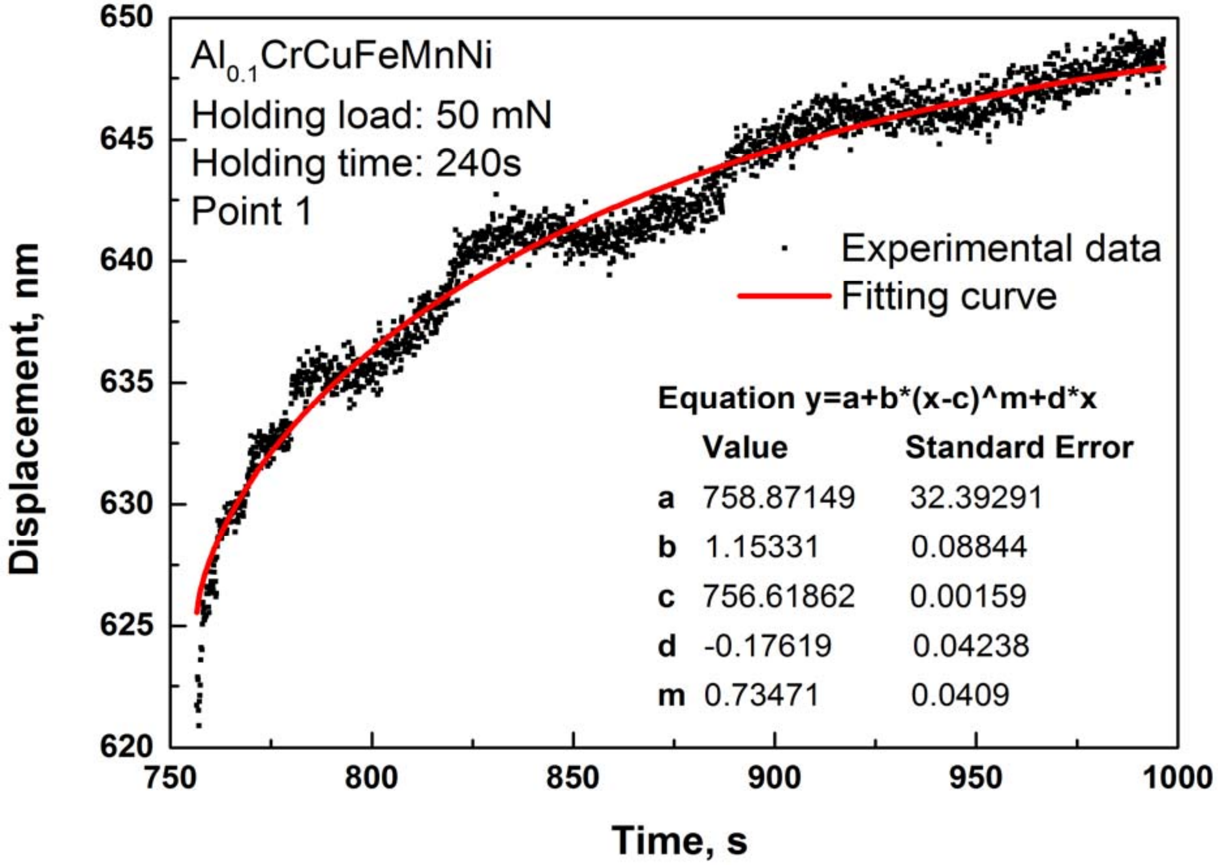
$$h(t) = h_i + \beta(t - t_i)^m + kt$$

where h is the displacement,
t is the time,
h_i, t_i, β, *m*, and *k* are fitting constants

H. Li and A. H. W. Ngan, "Size Effects of Nanoindentation Creep", Journal of Materials Research, Vol. 19, No. 2, pp. 513-522 (2004).

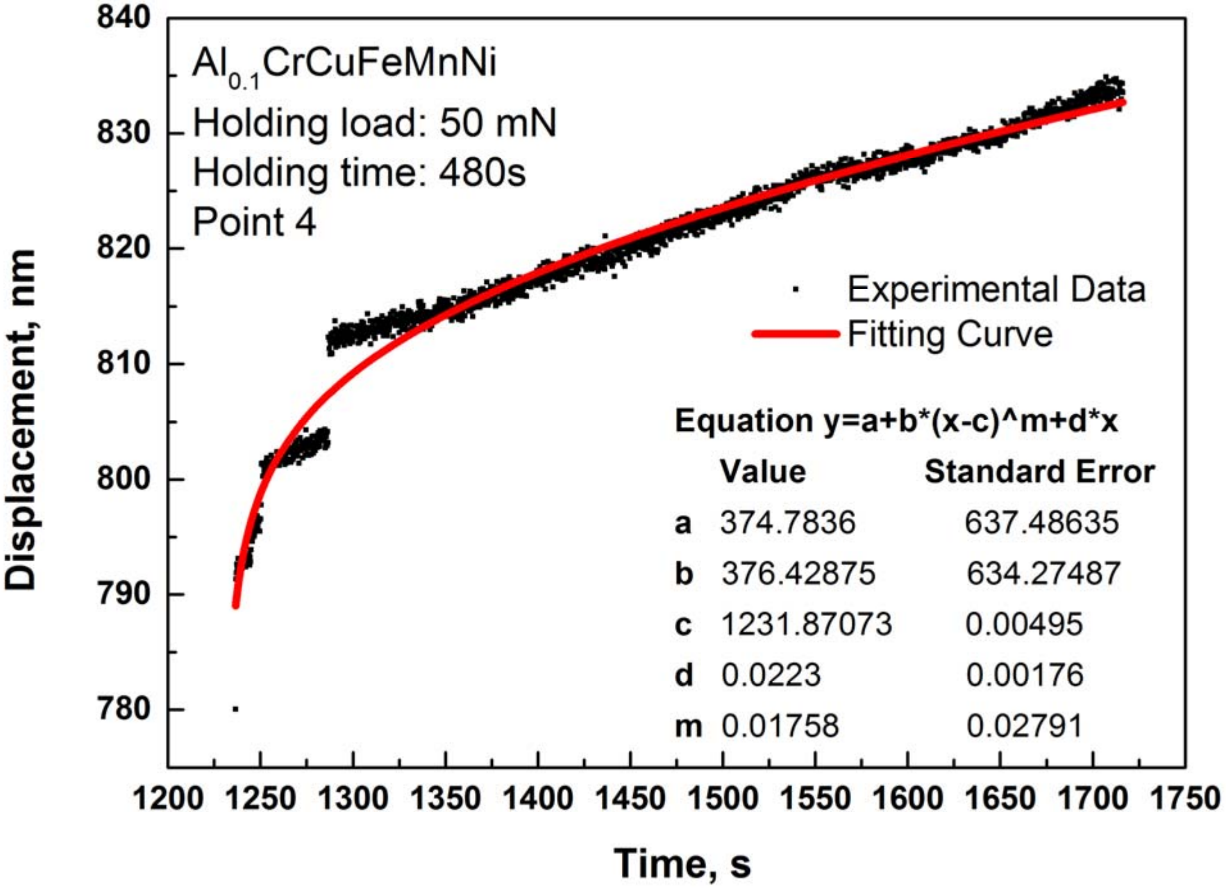
Nanoindentation Creep (Cont'd)

$$h(t) = h_i + \beta(t - t_i)^m + kt$$



Nanoindentation Creep (Cont'd)

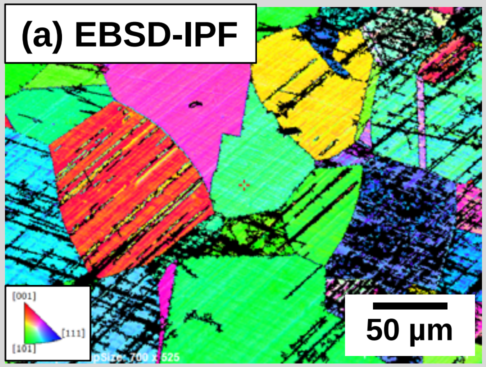
$$h(t) = h_i + \beta(t - t_i)^m + kt$$

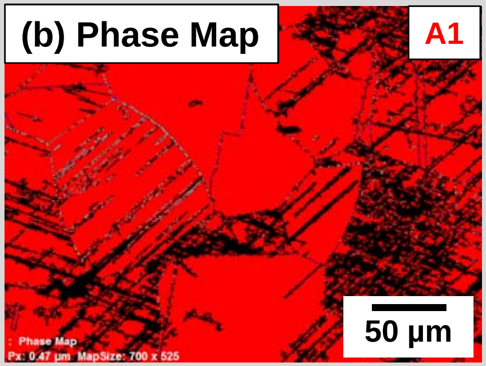


$Al_{0.3}CoCrFeNi$

As-forged

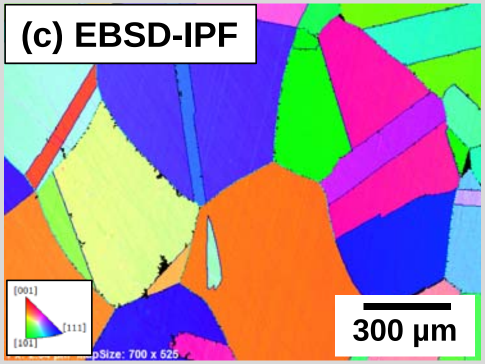
(as-cast + 1,250C/50h + 1,250C/50% reduction)

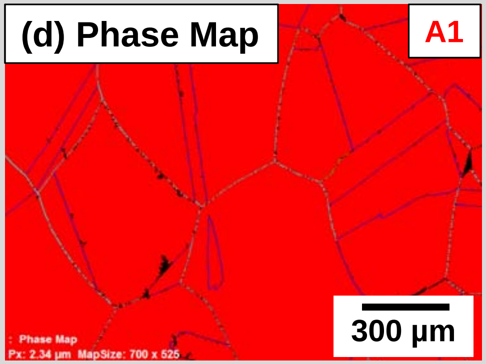




As-equilibrated

(1,250C/1,000h/WQ)



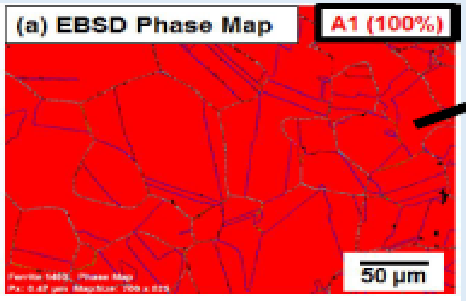


- Single-phase FCC remains but the grain size increases after equilibrium.

$Al_{0.3}CoCrFeNi$ (cont’d)

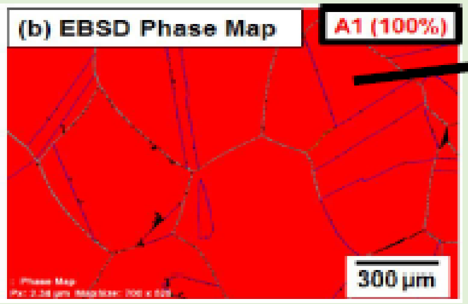
Atomic-Probe Tomography

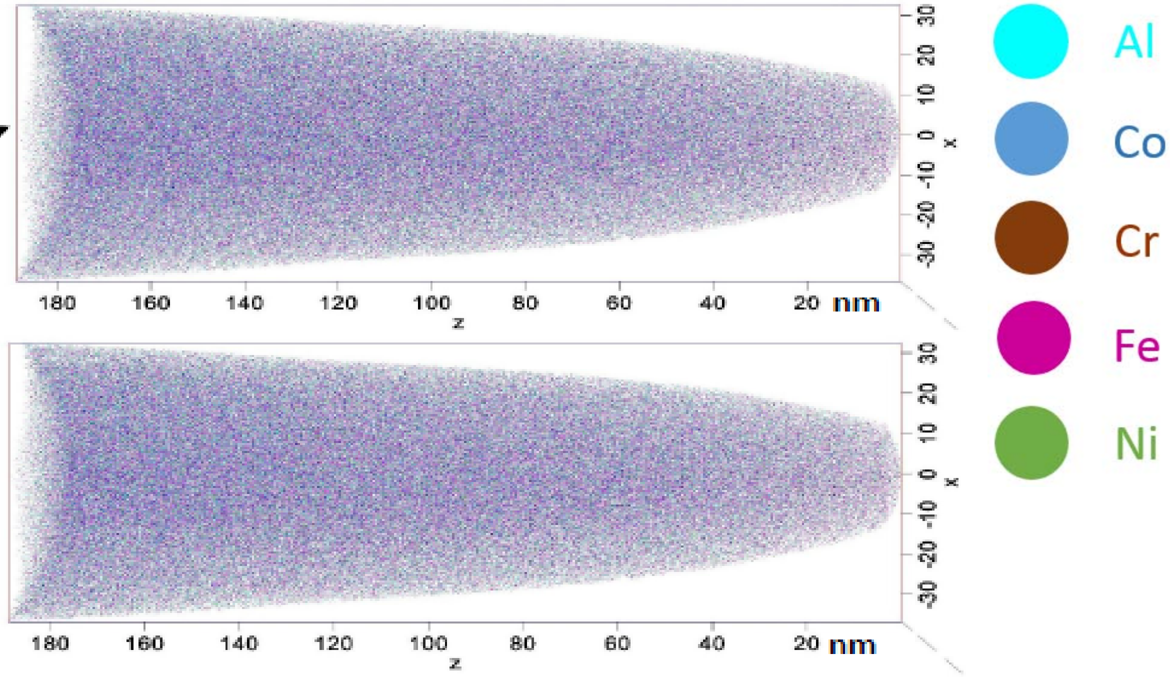
As-Fabricated



As-Equilibrated

(1,250ºC/1,000hrs/WQ)



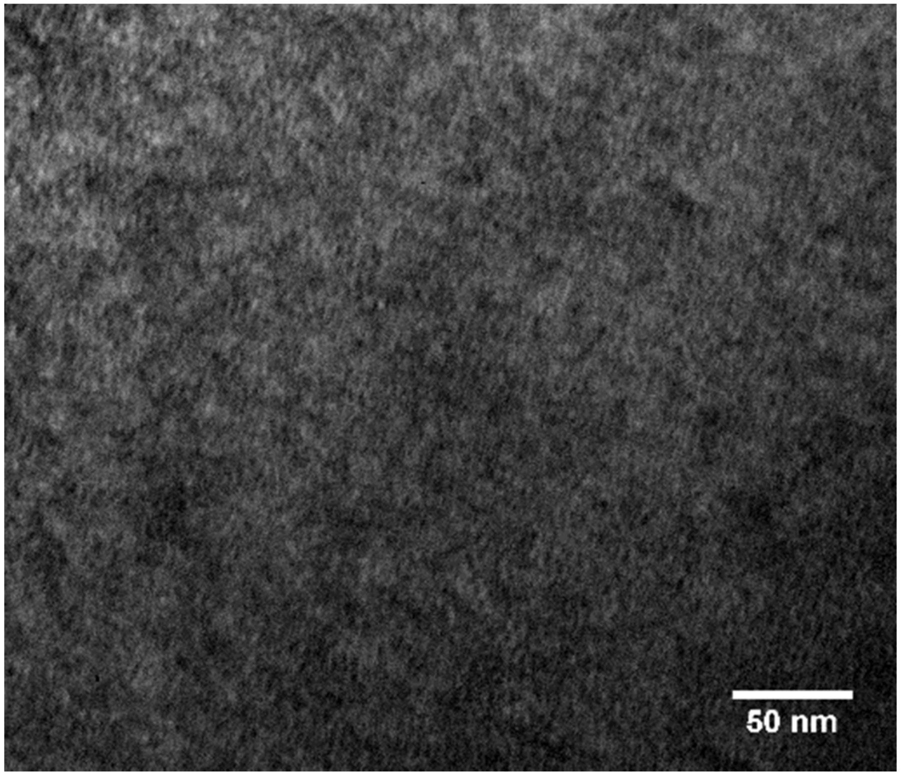


Chemical (at.%)	Al	Co	Cr	Fe	Ni
Nominal	6.977	23.256	23.256	23.256	23.256
As-Fabricated	7.040	23.297	23.402	23.436	22.824
As-Equilibrated	6.801	23.325	23.561	23.473	22.839

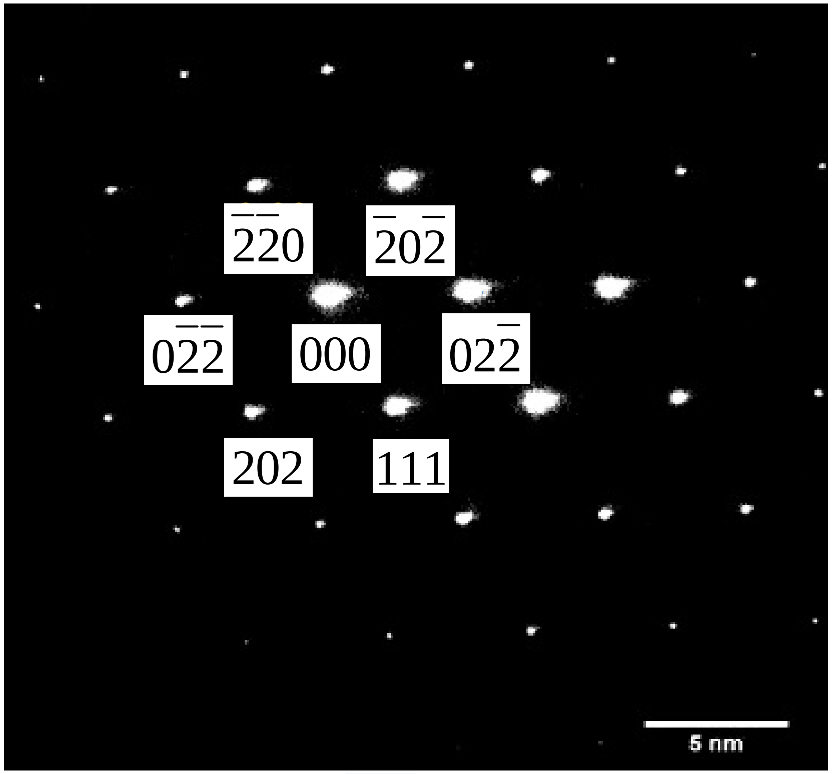
- A single-phase FCC structure was confirmed by the Atom Probe Tomography

Al$_{0.3}$CoCrFeNi

Transmission-Electron Microscopy



FCC structure

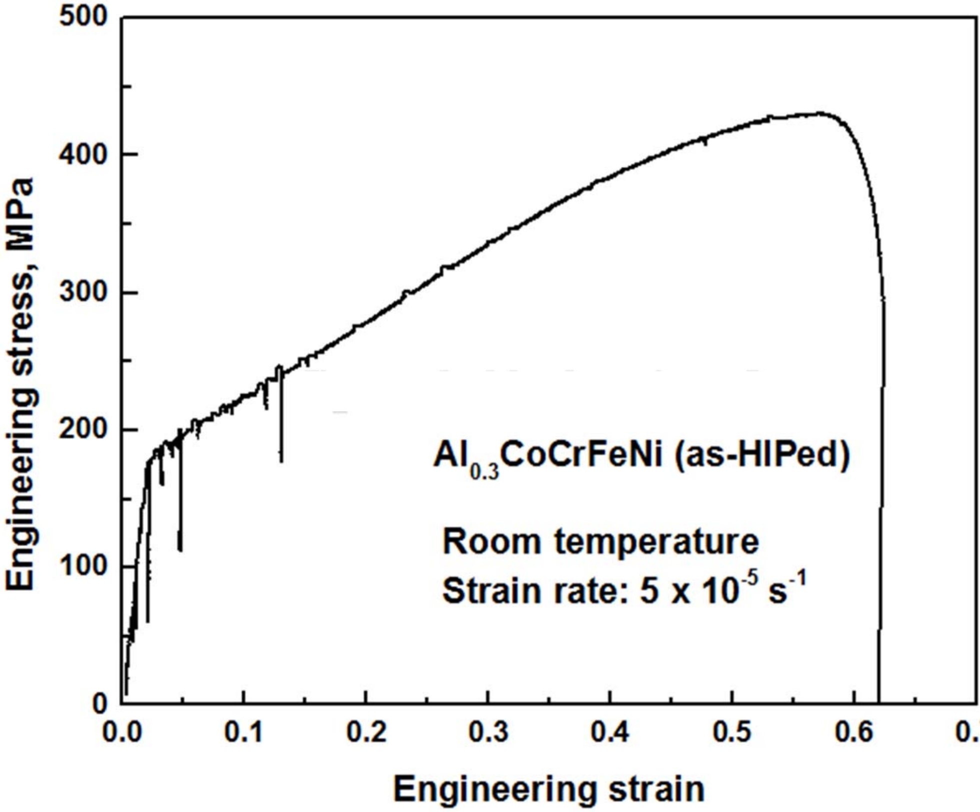


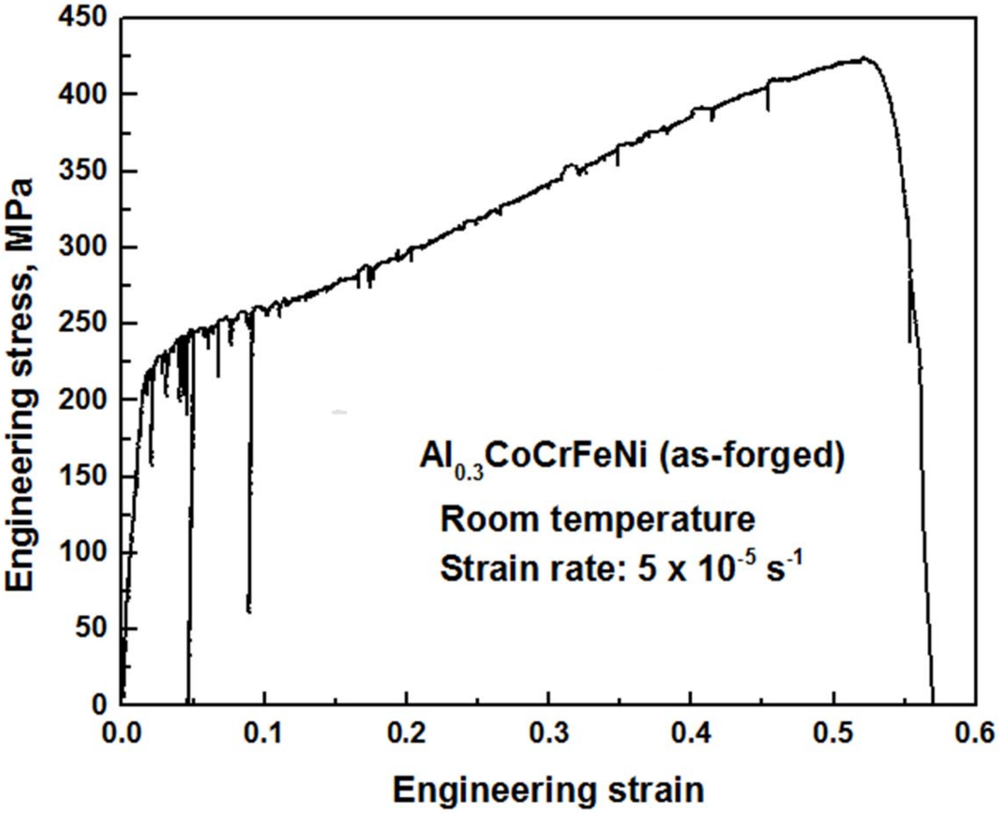
$\bar{1}11$

Hardness Values of $Al_{0.3}CoCrFeNi$ (as-forged) and $Al_{0.3}CoCrFeNi$ (as-equilibrated) HEAs, compared with all published single-phase FCC HEAs at room temperature

Alloy #	Hardness	Alloy #	Hardness
$Al_{0.3}CoCrFeNi$ (as-forged)	233	$Al_{0.1}CoCrFeNi$	113
$Al_{0.3}CoCrFeNi$ (as-equilibrated)	232	$Al_{0.3}CoCrFeNi$	123
CoCrCuFeNi	129	$Al_{0.4}CoCrFeNi$	126
$Al_{0.3}CoCrCuFeNi$	175	$Al_{0.2}CrCuFeNi_2$	162
$Al_{0.5}CoCrCuFeNi$	203	$Al_{0.3}CrCuFeNi_2$	169
CoCrFeNi	113	$Al_{0.4}CrCuFeNi_2$	201

Tension Tests (at Room Temperature)

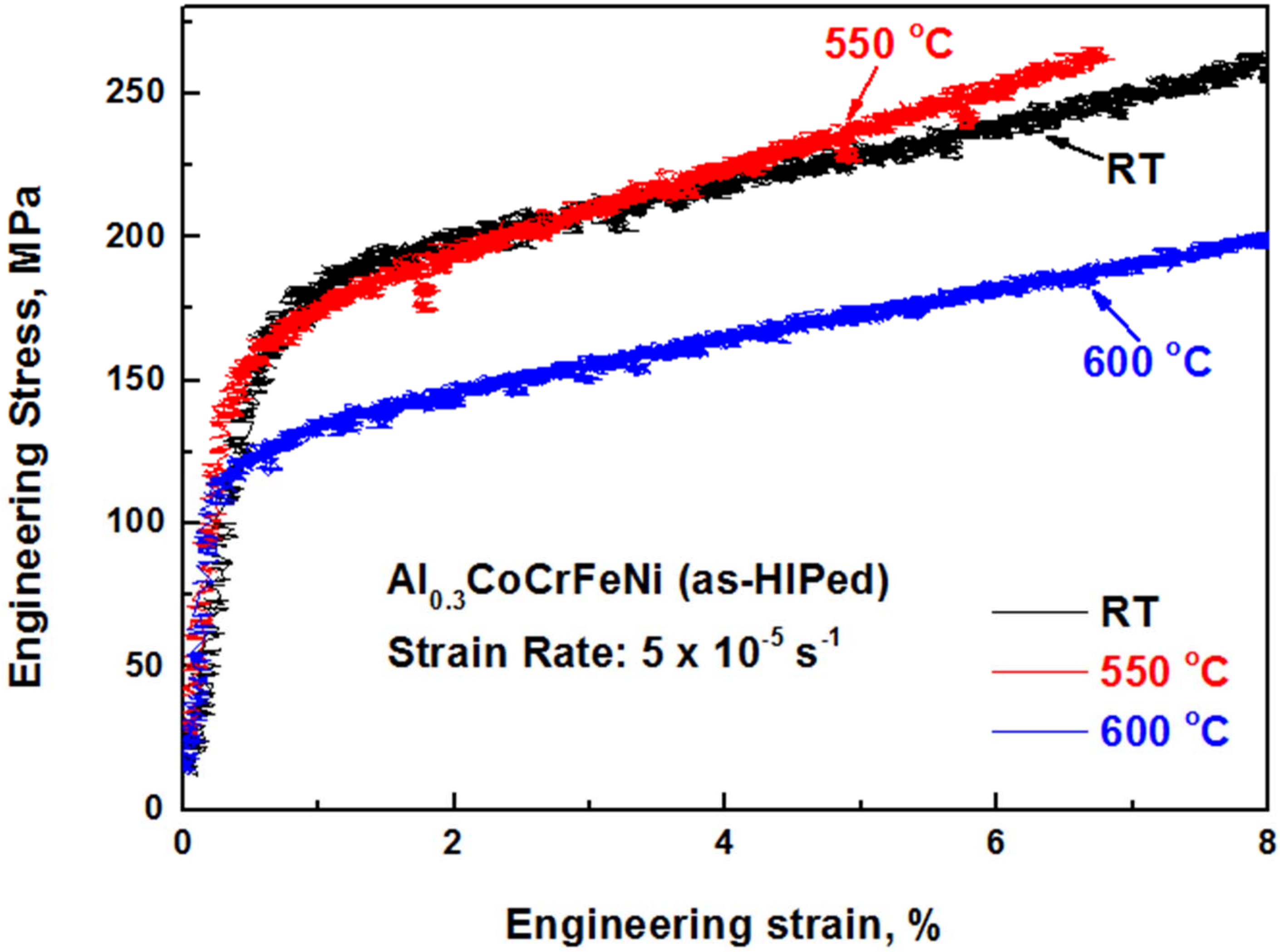




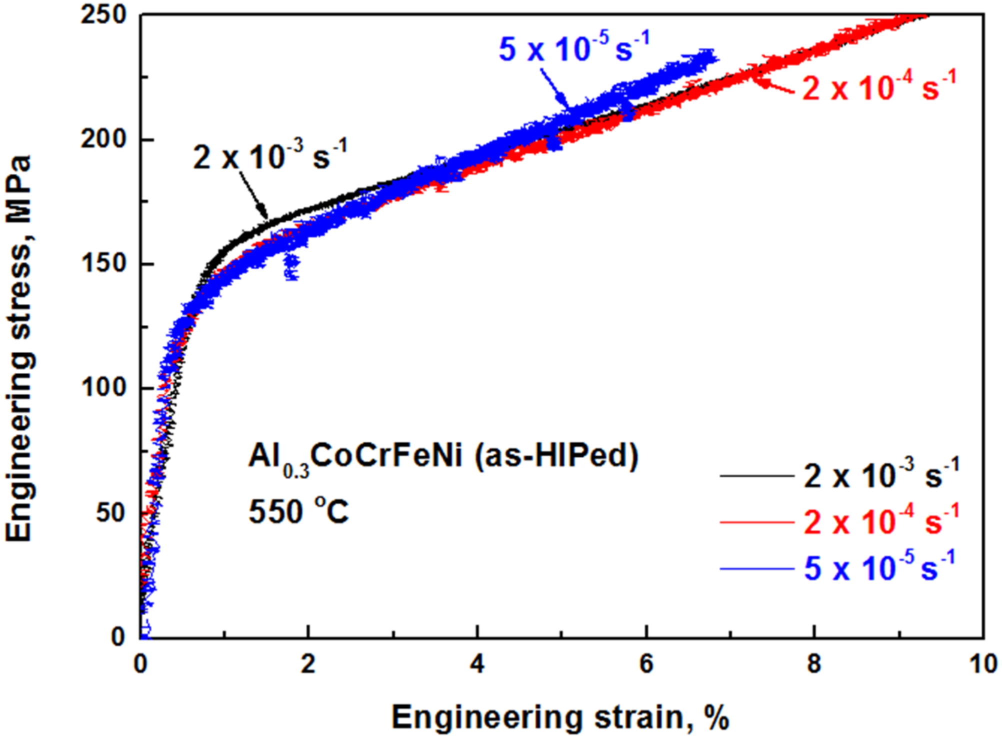
σ_y = 177 MPa, σ_{UTS} = 430 MPa, ε_f = 62 %

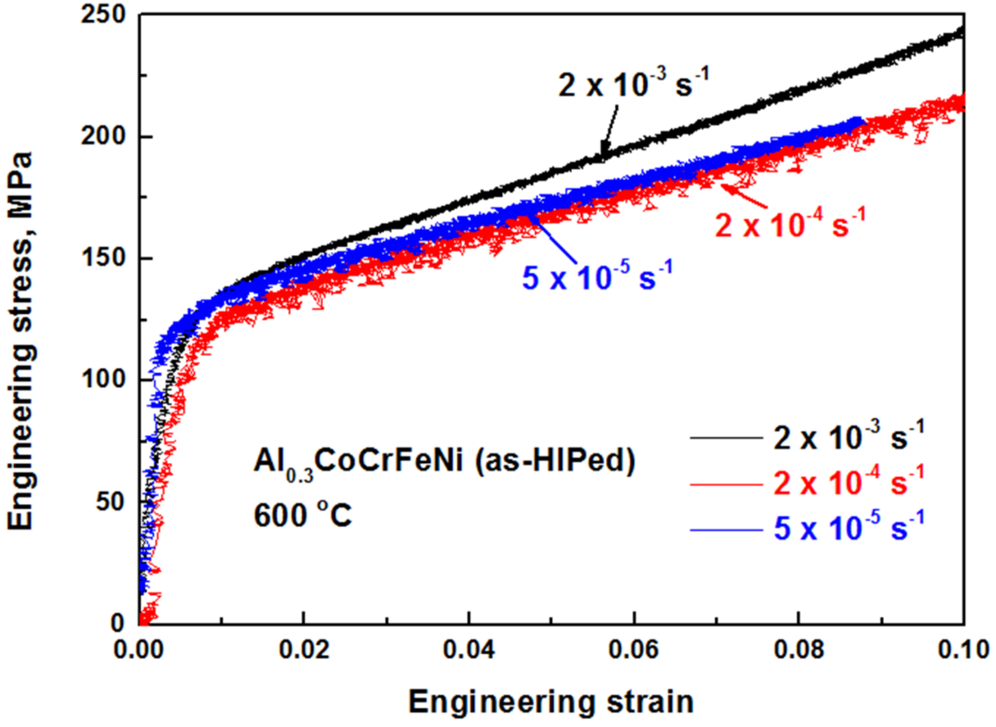
σ_y = 213 MPa, σ_{UTS} = 425 MPa, ε_f = 56 %

Compression Tests

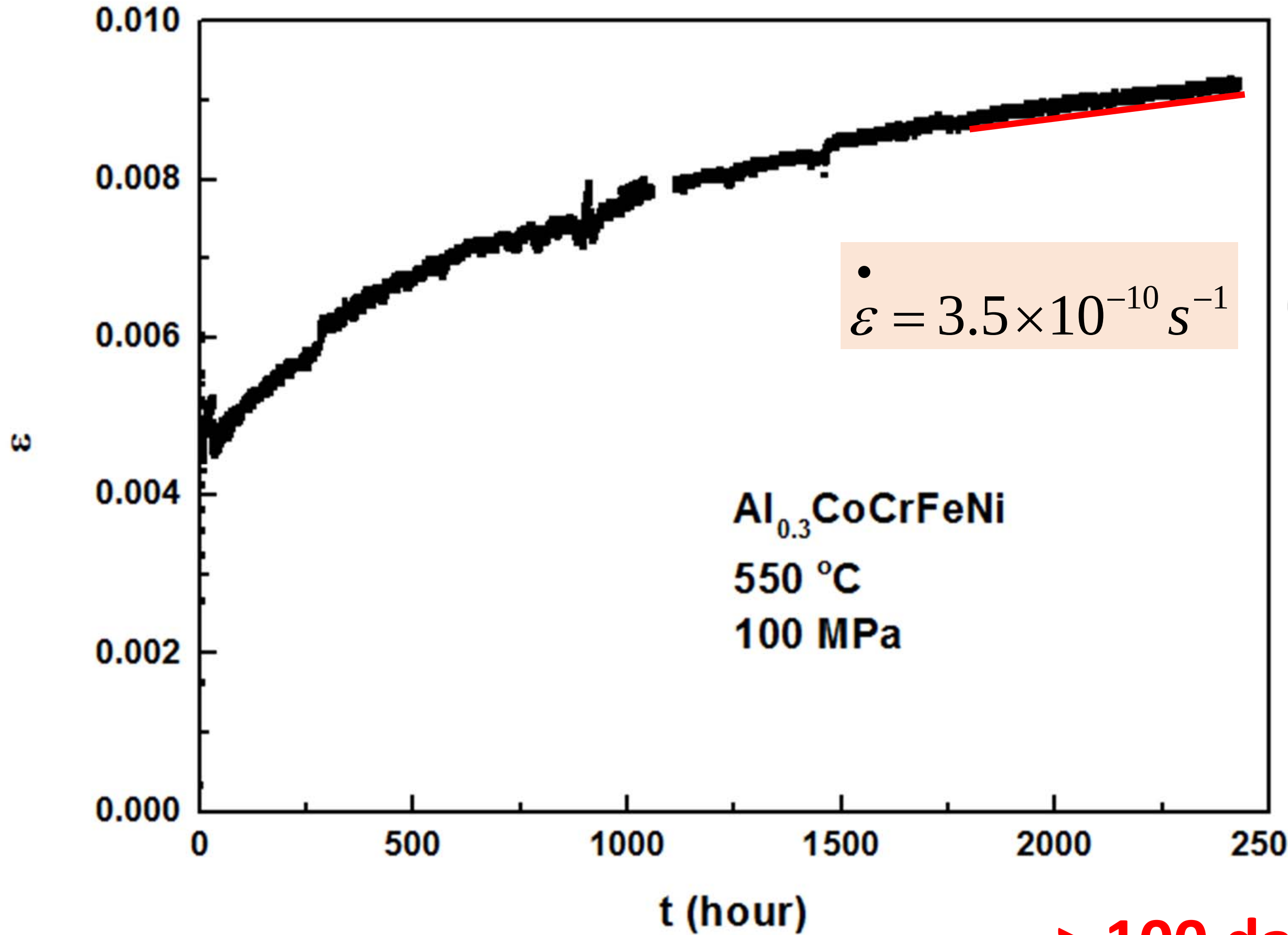


Compression Tests (Cont'd)

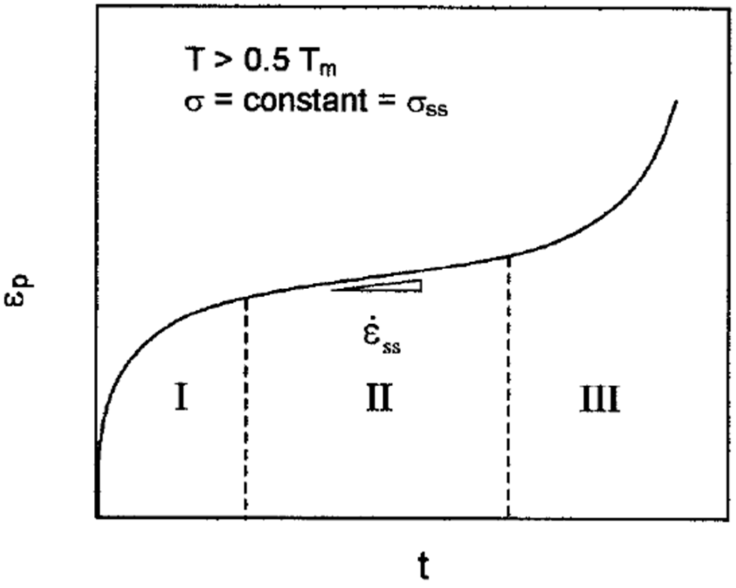




Conventional Creep Test at 550 °C and 100 MPa



$$\dot{\varepsilon} = 3.5\times10^{-10}\,s^{-1}$$

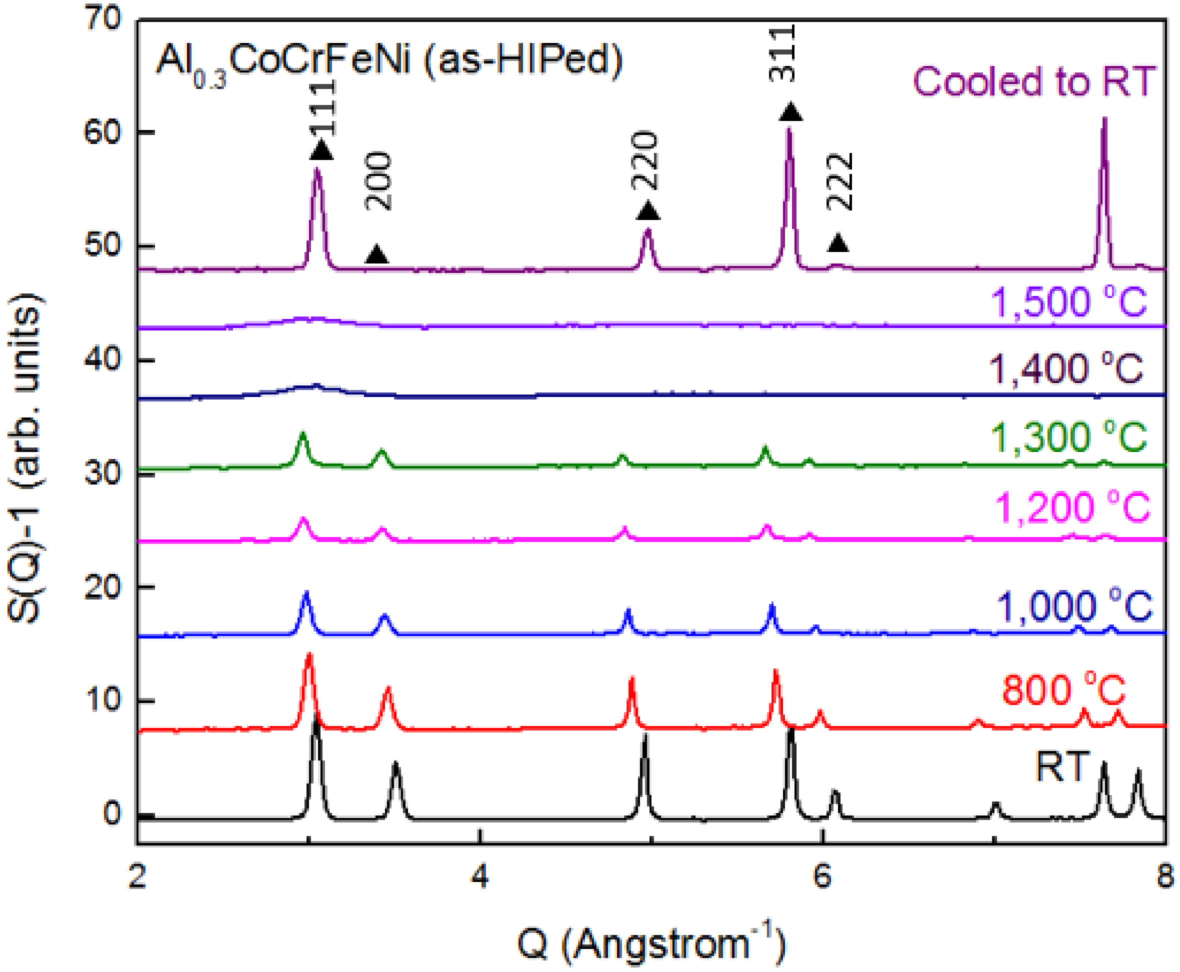


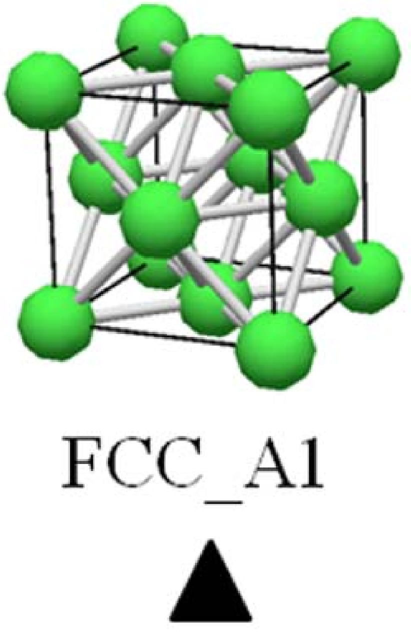
The creep-rate

$$\dot{\varepsilon} = \frac{d\varepsilon}{dt}$$

> 100 days

In-situ Neutron Levitation Results





Pure FCC phase

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[1] Guo XQ, Wu W, Wu PD, Qiao H, An K, Liaw PK. Scripta Materialia 2013;69:319.

[2] Jia HL, Muntele CI, Huang L, Li X, Li G, Zhang T, He W, Liaw PK. Intermetallics 2013;41:35.

[3] Ma SG, Zhang SF, Gao MC, Liaw PK, Zhang Y. Jom 2013;65:1751.

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[5] Tang Z, Gao MC, Diao HY, Yang TF, Liu JP, Zuo TT, Zhang Y, Lu ZP, Cheng YQ, Zhang YW, **Dahmen KA**, Liaw PK, Egami T. Jom 2013;65:1848.

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[8] Antonaglia J, Xie X, Schwarz G, Wraith M, Qiao JW, Zhang Y, Liaw PK, Uhl JT, **Dahmen KA**. Scientific reports 2014;4.

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[10] Chen SY, Yang X, **Dahmen KA**, Liaw PK, Zhang Y. Entropy 2014;16:870.

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[12] Huang EW, Qiao JW, Winiarski B, Lee WJ, Scheel M, Chuang CP, Liaw PK, Lo YC, Zhang Y, Di Michiel M. Scientific reports 2014;4.

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[13] Huang L, Fozo EM, Zhang T, Liaw PK, He W. Materials Science & Engineering C-Materials for Biological Applications 2014;39:325.

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[15] Jia HL, Liu FX, An ZN, Li WD, Wang GY, Chu JP, Jang JSC, Gao YF, Liaw PK. Thin Solid Films 2014;561:2.

[16] Wu W, Qiao H, An K, Guo XQ, Wu PD, Liaw PK. International Journal of Plasticity 2014;62:105.

[17] Yu PF, Feng SD, Xu GS, Guo XL, Wang YY, Zhao W, Qi L, Li G, Liaw PK, Liu RP. Scripta Materialia 2014;90-91:45.

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[21] Huang L, Zhu C, Muntele CI, Zhang T, Liaw PK, He W. Materials Science & Engineering C-Materials for Biological Applications 2015;47:248.

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[25] Santodonato LJ, Zhang Y, Feygenson M, Parish CM, Gao MC, Weber RJ, Neuefeind JC, Tang Z, and Liaw PK, Nature Communications 2015;6:5964.

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- The 9th International Conference on Bulk Metallic Glass (BMG-IX) 2012, Xiamen, China
  - Computational Thermodynamics Aided High-Entropy Alloy Design, C. Zhang, F. Zhang, S. L. Chen, W. S. Cao, Z. Tang, P. K. Liaw
- 2013 TMS Meeting , San Antonio, TX, USA, March 3-9, 2013
  - Automatic Fabrication of High-Entropy Alloys and Their Properties, Y. Yokoyama, X. Xie, J. Antonaglia, M. Hemphill, T. Zhi, T. Yuan, G. Wang, C. Tsai, J. Yeh, A. Chuang, **K. Dahmen**, P. K. Liaw (invited)
  - Extracting Materials Properties from Crackling Noise and Slip Avalanche Statistics of Slowly-Sheared Materials, **K. Dahmen**, X. Xie, J. Antonaglia, M. Laktionova, E. Tabachnikova, Z. Tang, J. Qiao, J. Greer, J. W. Yeh, J. Uh, P. Liaw
  - Non-Equilibrium and Equilibrium Phases in AlCoCrFeNi High-Entropy Alloys, Z. Tang, O. Senkov, C. Parish, L. Santodonato, D. Miracle, G. Wang, C. Zhang, F. Zhang, P. K. Liaw
  - Ordering Behavior in the Al(x)CoCrCuFeNi High-Entropy Alloys, L. Santodonato, Y. Zhang, M. Gao, C. Parish, M. Feygenson, Z. Tang, J. Neuefeind, R. Weber, P. K. Liaw
  - Computational Modeling of High-Entropy Alloys, M. Gao, D. Tafen, J. Hawk, Y. Wang, M. Widom, L. Santodonato, P. K. Liaw(invited)
  - Minor Phase and Defect Effects on Fatigue Behavior of Wrought Al0.5CoCrCuFeNi High-Entropy Alloys, Z. Tang, M. Hemphill, T. Yuan, G. Wang, J. Yeh, C. Tsai, P. K. Liaw
  - Phase Separation and Intermetallic Formation in "High-Entropy" Alloys, C. Parish, M. Miller, L. Santodonato, Z. Tang, P. K. Liaw.
  - Computational Thermodynamics Aided High-Entropy Alloy Design, C. Zhang, F. Zhang, S. Chen, W. Cao, J. Zhu, Z. Tang, P. K. Liaw
  - Statistical Fatigue-Life Modeling for High-Entropy Alloys, T. Yuan, M. Hemphill, Z. Tang, G. Wang, A. Chuang, C. Tsai, J. Yeh, P. K. Liaw (invited).

Presentations (Cont'd):

  - A Combinatorial Approach to the Investigation of Metal Systems that Form Both High Entropy Alloys and Bulk Metallic Glasses, B. Welk, P. K. Liaw, M. Gibson, H. Fraser

- 2014 TMS Meeting, San Diego, CA, USA, February 16-20, 2014
  - Aluminum Alloying Effects on Lattice Types, Microstructures, and Mechanical Behavior of High-entropy Alloys Systems, Z. Tang, M. Gao, H. Y. Diao, T. F. Yang, J. P. Liu, T. T. Zuo, Y. Zhang, Z. P. Lu, Y. Q. Cheng, Y. W. Zhang, **K. Dahmen**, P. K. Liaw, T. Egami.
  - The Influence of Cu and Al on the Microstructure, Mechanical Properties and Deformation Mechanisms in the High Entropy Alloys CrCoNiFeCu, CrCoNiFeAl1.5 and CrCoNiFeCuAl1.5, B. Welk, B. B. Viswanathan, M. Gibson, P. K. Liaw, and H. Fraser.
  - The Influence of Alloy Composition on the Interrelationship between Microstructure Mechanical Properties of High Entropy Alloys with BCC/B2 Phase Mixtures, B. Welk, D. Huber, J. Jensen, G. Viswanathan, R. Williams, P. K. Liaw, M. Gibson, D. Evans, and H. Fraser.
  - The Oxidation Behavior of AlCoCrFeNi High-entropy Alloy at 1023-1323K (750-1050oC), Wu Kai, W. S. Chen, C. C. Sung, Z. Tang, and P. K. Liaw.
  - Strain-rate Effects on the Structure Evolution of High Entropy Alloys, X. Xie, J. Antonaglia, J. P. Liu, Z. Tang, J. W. Qiao, G. Y. Wang, Y. Zhang, K. Dahmen, and P. K. Liaw.
  - Neutron diffraction studies on creep deformation behavior in a high-entropy alloy CoCrFeMnNi under high temperature and low strain rate, W. C. Woo, E. W. Huang, J. W. Yeh, P. K. Liaw, and H. Choo.
  - The Hot Corrosion Resistance Properties of AlxFeCoCrNi, **S. Z. Yang**, M. Habibi, L. Wang, S. M. Guo, Z. Tang, P. K. Liaw, L. X. Tan, C. Guo, and M. Jackson.
  - Using the Statistics of Serrations in the Stress Strain Curves to Extract Materials Properties of Slowly-sheared High Entropy Alloys, **Karin Dahmen**, X. Xie, J. Antonaglia, M. Laktionova, E. Tabachnikova, J. W. Qiao, J. W. Yeh, C. W. Tsai, J. Uh, and P. K. Liaw.

Presentations (Cont’d):

  - Environmental-temperature Effect on a Ductile High-entropy Alloy Investigated by In Situ Neutron-diffraction Measurements, E. W. Huang, C. Lee, D. J. Yu, K. An, P. K. Liaw, and J. W. Yeh.
  - Mechanical Behavior of an Al0.1CoCrFeNi High Entropy Alloy, M. Komarasamy, N. Kumar, Z. Tang, **R. Mishra**, and P. K. Liaw.
  - Characterizing Multi-component Solid Solutions Using Order Parameters and the Bragg-Williams Approximation, L. Santodonato, and P. K. Liaw.
  - Ultra Grain Refinement in High Entropy Alloys, N. Tsuji, I. Watanabe, N. Park, D. Terada, A. Shibata, Y. Yokoyama, P. K. Liaw.
  - Nanostructure Evolution through High-pressure Torsion and Recrystallization in a High-entropy CrMnFeCoNi Alloy, N. Park, A. Shibata, D. Terada, Y. Yokoyama, P. K. Liaw, and N. Tsuji.
  - Distinguished Work-hardening Capacity of a Ti-based Metallic Glass Matrix Composite upon Dynamic Loading, J. W. Qiao, H. J. Yang, Z. H. Wang, and P. K. Liaw.
- The 10th International Conference on Bulk Metallic Glass 2014, Shanghai, China, University of Science and Technology, Beijing, June 6-16, 2014
  - Characterization of Serrated Flows in BMG and HEAs, X. Xie, S. Y. Chen, J. Auto, J. P. Liu, J. W. Qiao, P. K. Liaw (invited).
- National Institute of Materials Science, Japan, 2014
  - Fatigue Behavior of BMG and HEAs, X. Xie, G. Y. Wang, P. K. Liaw.
- University of Science and Technology, Beijing, China, June 9, 2014 (Invited)
  - Characterization of Serrated Flows in High-Entropy Alloys and Bulk-Metallic Glasses, P. K. Liaw.
- Beihang University, Beijing, China, June 10, 2014 (Invited)
  - Characterization of Serrated Flows in High-Entropy Alloys and Bulk-Metallic Glasses, P. K. Liaw.

Presentations (Cont'd):

- National Institute of Materials Science, Japan, June 23-24, 2014 (Keynote)
    - Fatigue Behavior of Bulk Metallic Glasses and High Entropy Alloys, Peter K. Liaw.
- 2014 Gordon Research Conferences, Hong Kong, China, July 20-25, 2014
    - Loading Condition Effects on the Serrated Flows in Bulk Metallic Glasses (BMGs) (poster), X. Xie, J. Antonaglia, J. W. Qiao, Y. Zhang, G. Y. Wang, **K. A. Dahmen**, and P. K. Liaw.
    - Characterization of Deformation Dynamics in Bulk Metallic Glasses (BMGs) (Invited), X. Xie, J. Antonaglia, J. W. Qiao, Y. Zhang, G. Y. Wang, Y. Yokoyama, **K. A. Dahmen**, and P. K. Liaw.
- Central South University, Changsha, Hunan, China, July 26th, 2014 (Invited)
    - Serration Behaviors of High Entropy Alloys and Bulk Metallic Glasses, X. Xie, J. Antonaglia, J. W. Qiao, Y. Zhang, G. Y. Wang, Y. Yokoyama, **K. A. Dahmen**, and P. K. Liaw.
- Dalian University of Technology, Dalian, Liaoning, China, July 28th, 2014 (Invited)
    - Serration Behaviors of High Entropy Alloys and Bulk Metallic Glasses, X. Xie, J. Antonaglia, J. W. Qiao, Y. Zhang, G. Y. Wang, Y. Yokoyama, **K. A. Dahmen**, and P. K. Liaw.
- University of California, Los Angeles, California, US, October 17th, 2014 (Invited)
    - Serration Behaviors of High Entropy Alloys and Bulk Metallic Glasses, X. Xie, J. Antonaglia, J. W. Qiao, Y. Zhang, G. Y. Wang, Y. Yokoyama, **K. A. Dahmen**, and P. K. Liaw.
- Yale University, New Haven, Connecticut, US, October 10th, 2014 (Invited)
    - Serration Behaviors of High Entropy Alloys and Bulk Metallic Glasses, X. Xie, J. Antonaglia, J. W. Qiao, Y. Zhang, G. Y. Wang, Y. Yokoyama, **K. A. Dahmen**, and P. K. Liaw.
- University of Cambridge, Cambridge, United Kingdom, December 8th, 2014 (Invited)
    - Serration Behaviors of High Entropy Alloys and Bulk Metallic Glasses, X. Xie, J. Antonaglia, J. W. Qiao, Y. Zhang, G. Y. Wang, Y. Yokoyama, **K. A. Dahmen**, and P. K. Liaw.

Presentations (Cont'd):

- 2015 TMS Meeting, Orlando, FL, USA, March 15-19, 2015
    - On the Friction Stress and Hall-Petch Coefficient of a Single Phase Face-Centered-Cubic High Entropy Alloy Al0.1FeCoNiCr (Invited), Nilesh Kumar, Mageshwari Komarasamy, Zhi Tang, Rajiv Mishra, and Peter Liaw.
    - Strength and Deformation of Individual Phases in High-Entropy Alloys, A. Giwa, Haoyan Diao, Xie Xie, S. Y. Chen, Zhi Tang, Karin Dahmen, and Peter Liaw.
    - Al-Co-Cr-Fe-Ni Phase Equilibria and Properties, Zhi Tang, Oleg Senkov, Chuan Zhang, Fan Zhang, Carl Lundin, and Peter Liaw.
    - Fatigue Behavior of an Al0.1CoCrNiFe High Entropy Alloy, Bilin Chen, Xie Xie, Shuying Chen, Ke An, and Peter Liaw.
    - Modeling Plastic Deformation and the Statistics of Serrations in the Stress versus Strain Curves of Bulk Metallic Glasses and Other Materials (Invited), **Karin Dahmen**, James Antonaglia, Wendelin Wright, Xiaojun Gu, Xie Xie, Michael LeBlanc, Junwei Qiao, Yong Zhang, Todd Hufnagel, Jonathan Uhl, and Peter Liaw.
    - Deformation Twinning in the High-Entropy Alloy Induced by High Pressure Torsion at Room Temperature, Gong Li, P.F. Yu, P.K. Liaw, and R.P. Liu.
    - Microstructures and Mechanical Behavior of Multi-Component AlxCrCuFeMnNi High-Entropy Alloys, Haoyan Diao, Zhinan An1; Xie Xie, Gongyao Wang, Chuan Zhang, Fan Zhang, Guangfeng Zhao, Fuqian Yang, **Karin Dahmen**, and Peter Liaw.
    - The Characterization of Serrated Plastic Flow in High Entropy Alloys, Shuying Chen, Xie Xie, James Antonaglia, Junwei Qiao, Yong Zhang, **Karin Dahmen**, and Peter Liaw.
    - A Model for the Deformation Mechanisms and the Serration Statistics of High Entropy Alloys, **Karin Dahmen**, Bobby Carroll, Xie Xie, Shuying Chen, James Antonaglia, Braden Brinkman, Michael LeBlanc, Marina Laktionova, Elena Tabachnikova, Zhi Tang, Junwei Qiao, Jien Wei Yeh, Chi Lee, Che Wei Tsai, Jonathan Uhl, and Peter Liaw.

Presentations (Cont’d):

- Segregation and Ti-Zr-Hf-Ni-Pd-Pt High Entropy Alloy under Liquid State, Y. Yokoyama, Norbert Mattern, Akitoshi Mizuno, Gongyao Wang, and Peter Liaw.
- Computational-Thermodynamics-Aided Development of Multiple-Principal-Component Alloys (Invited), Chuan Zhang, Fan Zhang, Shuanglin Chen, Weisheng Cao, Jun Zhu, Zhi Tang, Haoyan Diao, and Peter Liaw.
- Sputter Deposition Simulation of High Entropy Alloy via Molecular Dynamics Methodology (Invited), Yunche Wang, Chun-Yi Wu, Nai-Hua Yeh, and Peter Liaw.

Conclusions

- **AlxCrCuFeMnNi HEAs are multi-phase HEAs**
  - **The phase types are strongly dependent on aluminum ratio**
  - **The phase-segregation behavior of Al0.8CrCuFeMnNi is similar to that of $Al_{1.3}$CrCuFeCoNi (Al-Ni, Cr-Fe, and Cu-Cu)**
  - **The phases of Al0.1CrCuFeMnNi are stable at high temperatures up to 1,200 °C. Above 1,200 °C , one Cu-rich FCC disappears.**

- **The mechanical behavior is studied at different temperatures and strain rates**
  - **As the aluminum content increases, yielding stress increases and compression plasticity decreases**
  - **The mechanical behavior at room temperature is insensitive to strain rates**
  - **The compressive behavior is sensitive to temperature**

Conclusions (Cont'd)

Nanoindentation creep of $Al_{0.1}CrCuFeMnNi$ under fixed loads of 20, 35, and 50 mN, and holding times ranging from 10 s to 480 s was characterized.

- The pop-in phenomenon occurs and can be more frequently and regularly, as the indentation load is greater than 35 mN.
- The indenter displacement (h) versus time (t) curve at a constant indentation load was fitted by the empirical law,

$$h(t) = h_i + \beta(t - t_i)^m + kt$$

- If serrations happen, the empirical law doesn't apply.

Conclusions (Cont’d)

$Al_{0.3}CoCrFeNi$

- **It is a single-phase FCC HEA**
- **The mechanical behavior is the best among the presently published single-phase FCC HEAs.**
- **Below 550 °C, the mechanical behavior is stable.**
- **At 550 °C and 100 MPa, the creep rate is relatively low.**
- **The FCC phase of $Al_{0.3}CoCrFeNi$ is stable at high temperatures up to 1,300 °C. The material melts at 1,400 °C.**

Future Work

- The comparison between AlxCrCuFeMnNi and AlxCoCrFeNi HEAs will be qualitatively and quantitatively studied.
- In-situ tension synchrotron diffraction data will be utilized to study the elastic and plastic behavior of Al0.3CoCrFeNi.
- More conventional creep tests (at higher temperatures and loads) and related microstructures will be studied.
- Ab-initio molecular-dynamics (AIMD) calculations will be conducted to obtain the pair distribution functions that can be compared with the neutron results.

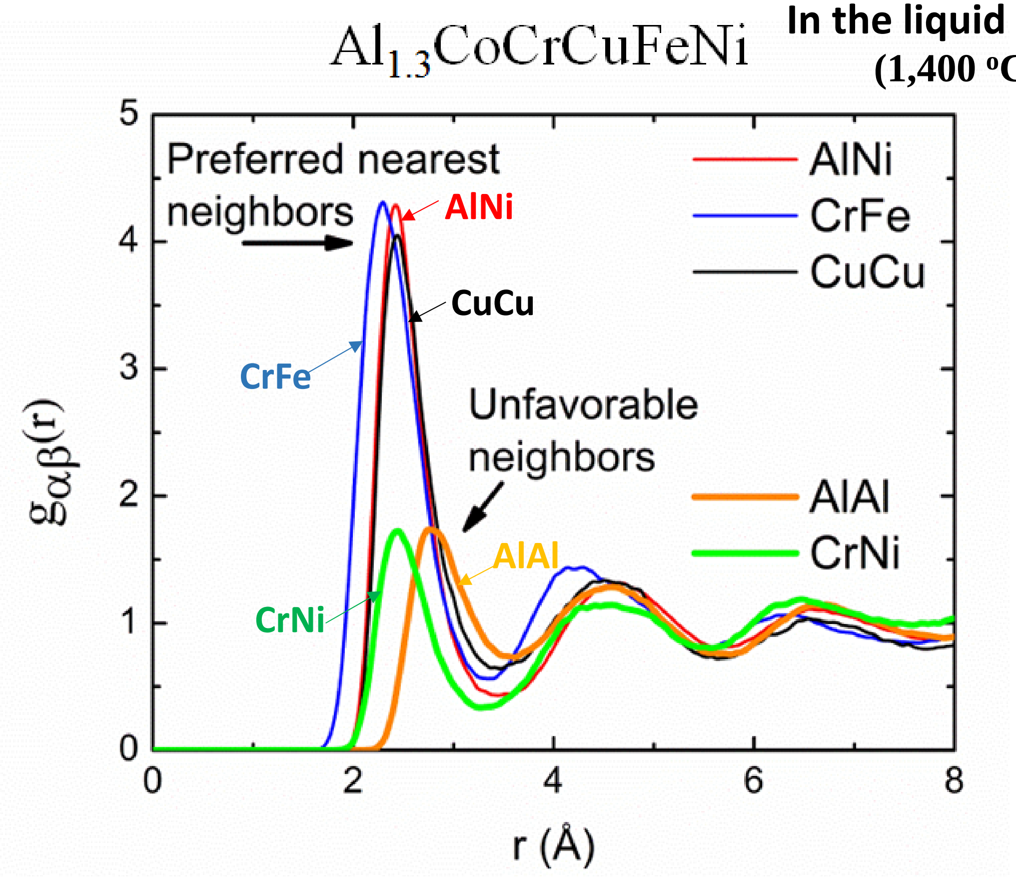
Thank you for your attention.
Your comments are welcome and appreciated.

Microstructures – Al1.3CoCrCuFeNi

❑Phase-segregation behavior

- Selected partial-pair-correlation functions, $g_{ab}(r)$, indicate that some pairs (e.g., Al-Ni, Cr-Fe, and Cu-Cu) are much more likely to be found as nearest neighbors than others (e.g., Al-Al and Cr-Ni).
- Such preferred nearest-neighbor pairing in the liquid phase is consistent with the formation of a B2-ordered solid-solution primary phase, which is supported by the presence of superstructure peaks in the high-temperature diffraction data

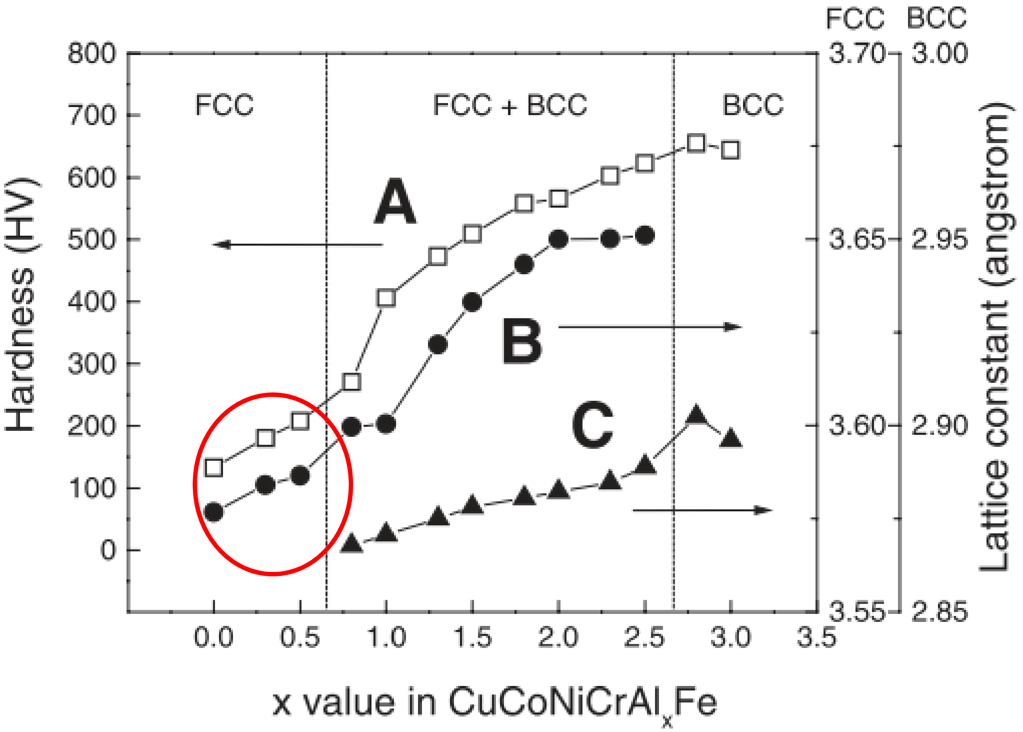
In the liquid state (1,400 ºC)

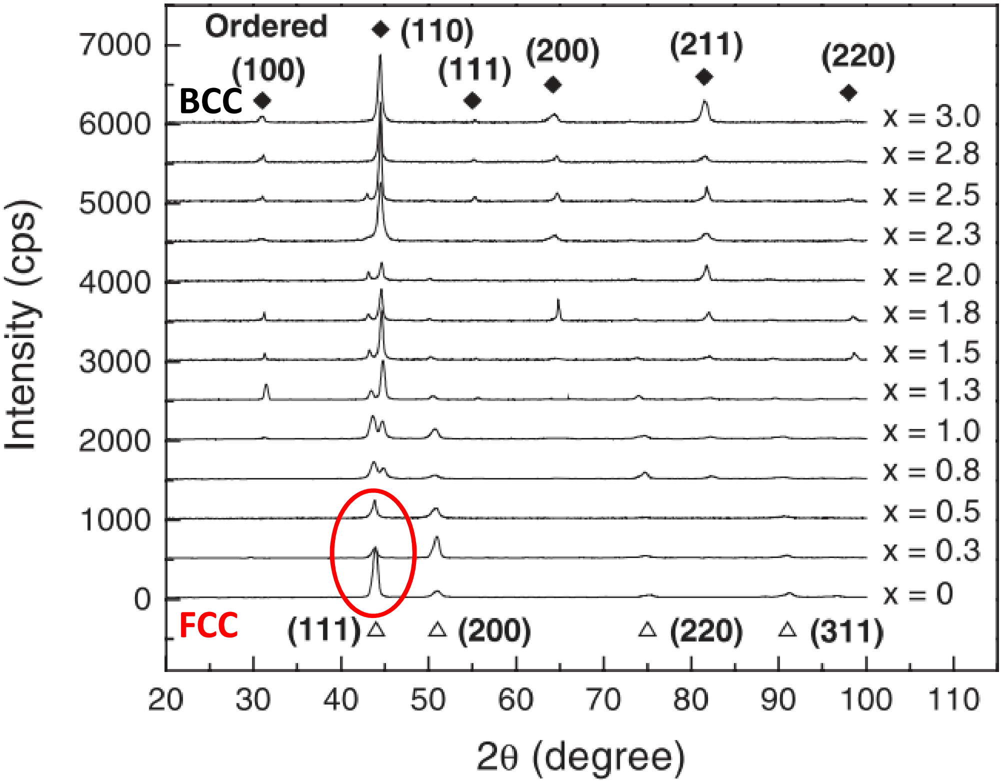


Ab-initio Molecular-dynamics (AIMD) Studies

L. J. Santodonato, Y. Zhang, M. Feygenson, C. M. Parish, M. C. Gao, R. J. Weber, J. C. Neuefeind, Z. Tang, and P. K. Liaw, *Nature Communications*, 2015, 6, pp. 5964.

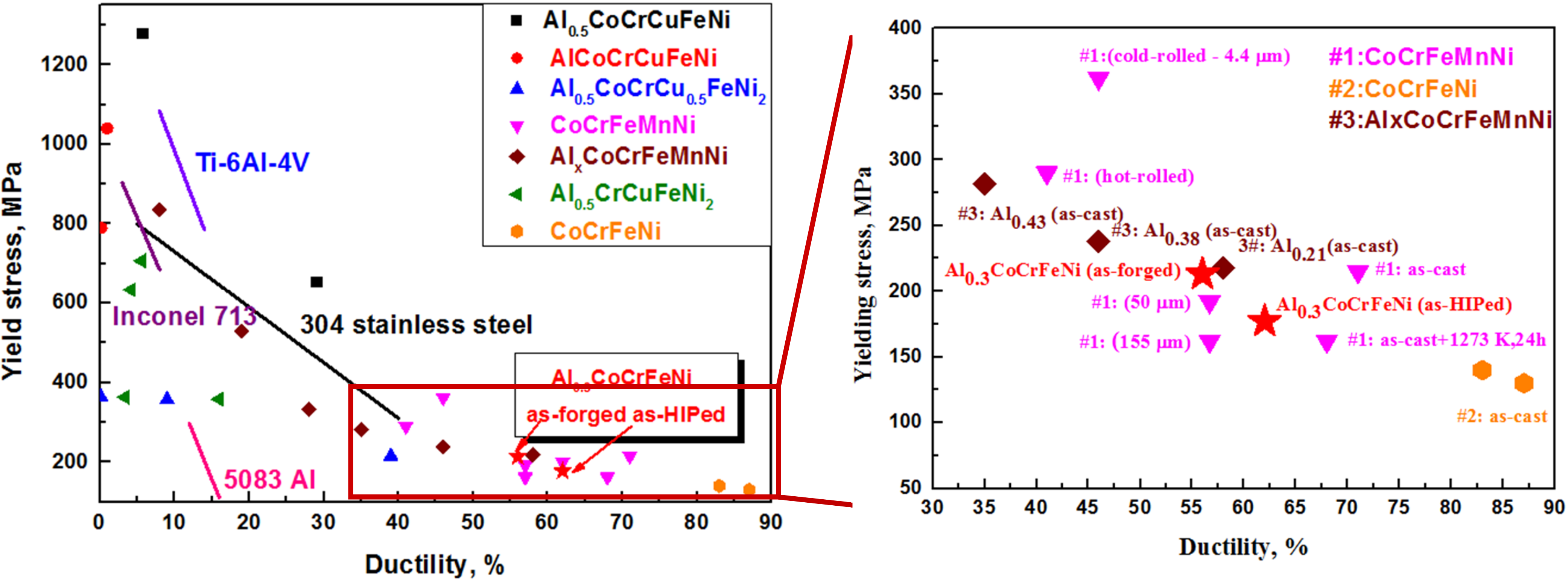
Microstructural Characterizations



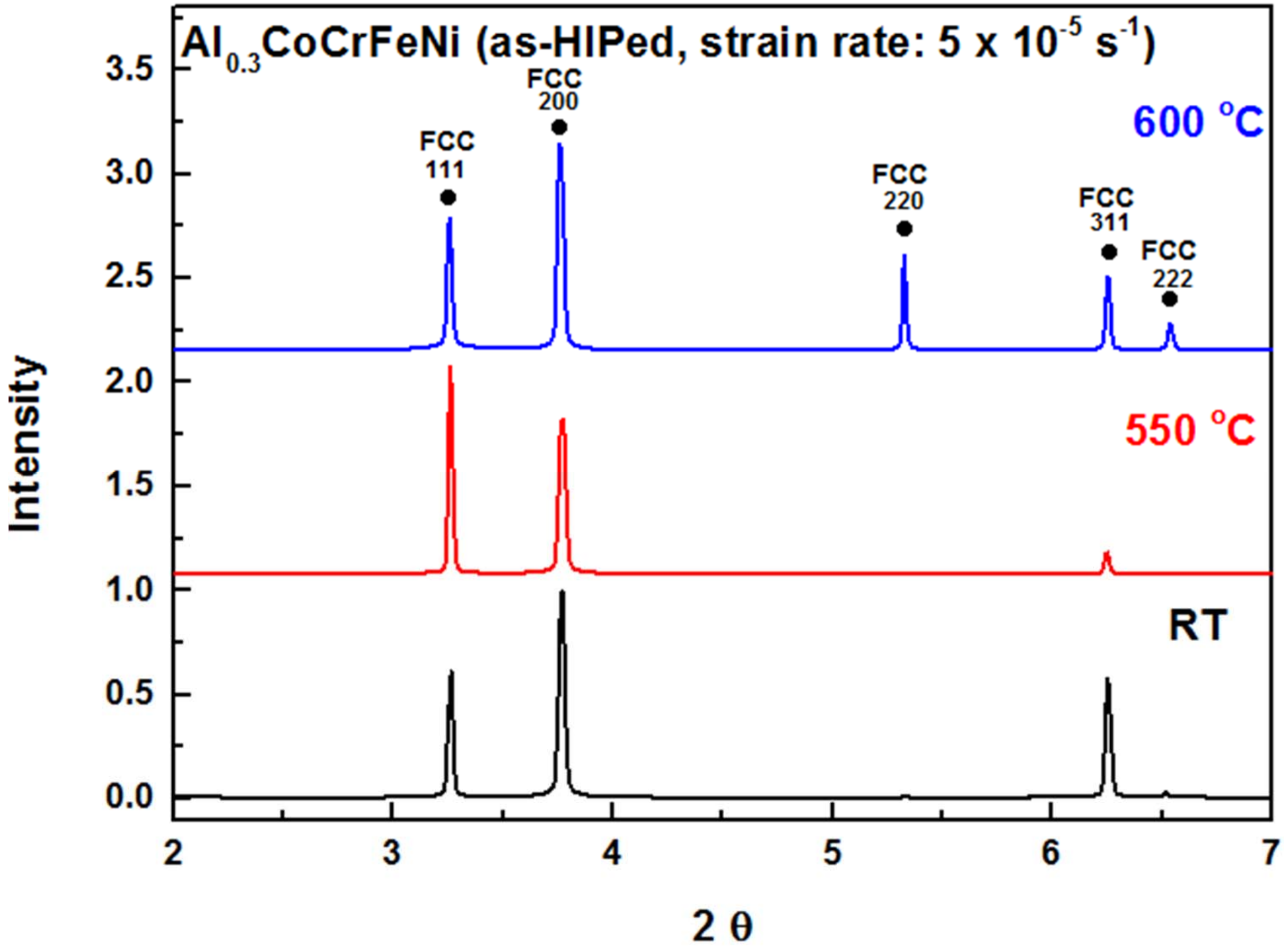


J. W. Yeh, S. K. Chen, S. J. Lin, J. Y. Gan, T. S. Chin, T. T. Shun, C. H. Tsau, and S. Y. Chang, Advanced Engineering Materials 6, 299 (2004).

Tension tests (at room temperature, Cont'd)



Compression tests (Cont’d)



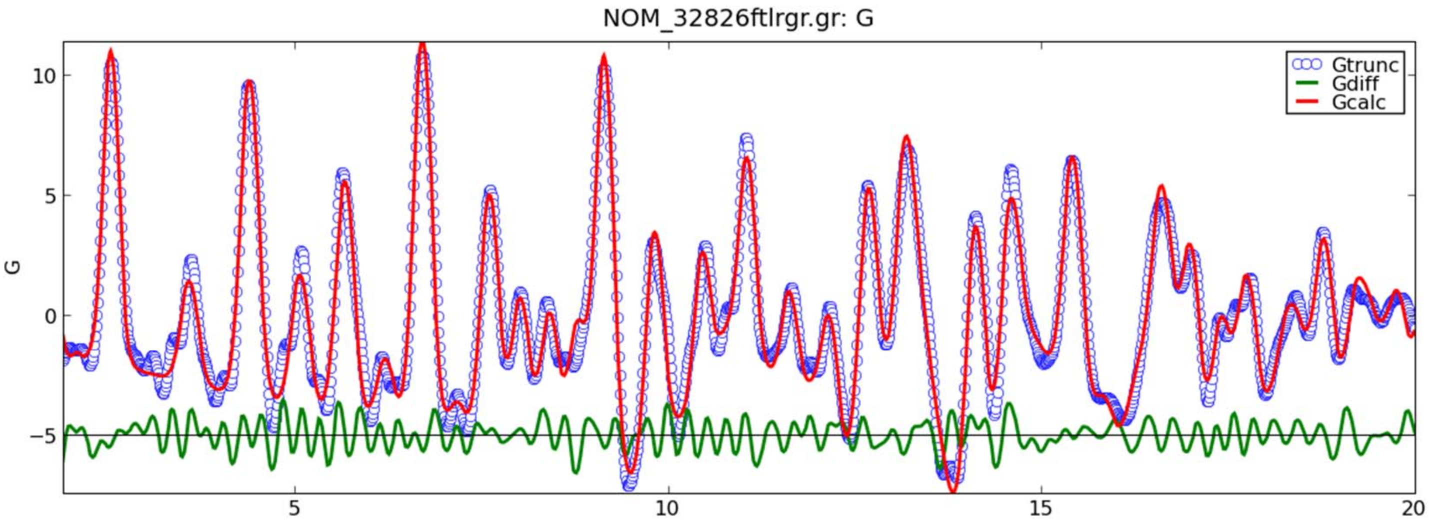
In-situ Neutron Levitation Results

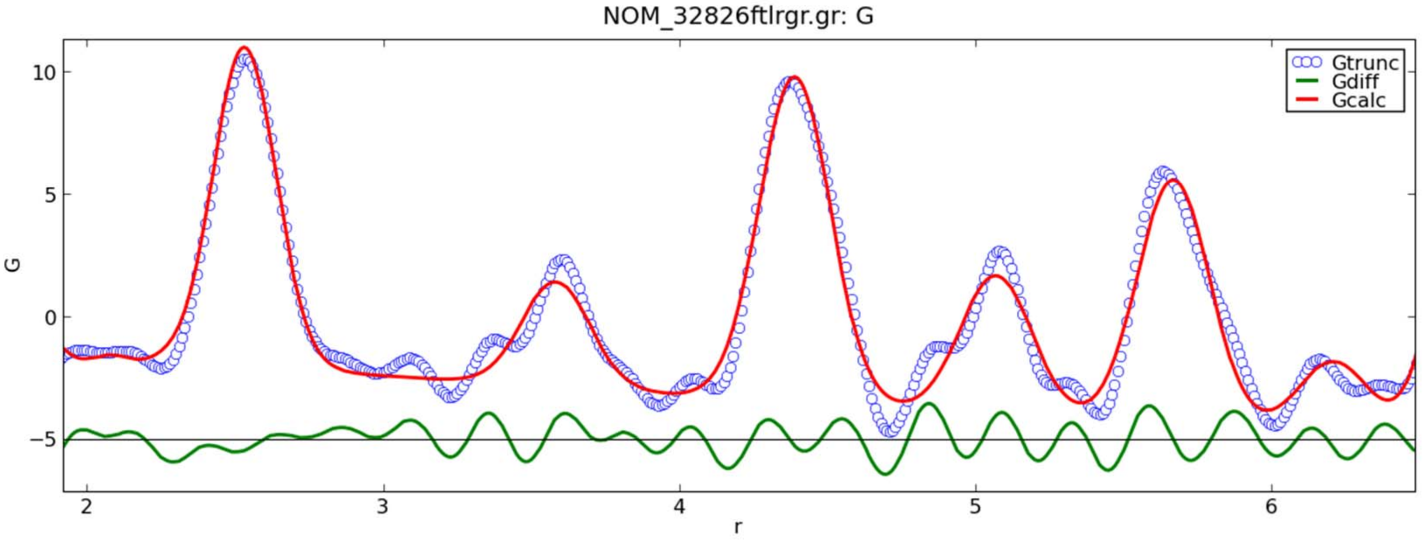
The reduced pair distribution function, G(r), is obtained through Fourier transformation of the X-ray structure function, S(Q):

$$G(r) = \frac{2}{\pi} \int_0^\infty Q[S(Q) - 1] \sin(Qr) dQ$$

r is the inter-atomic distance, and Q is the scattering vector

PDF studies of Neutron Results

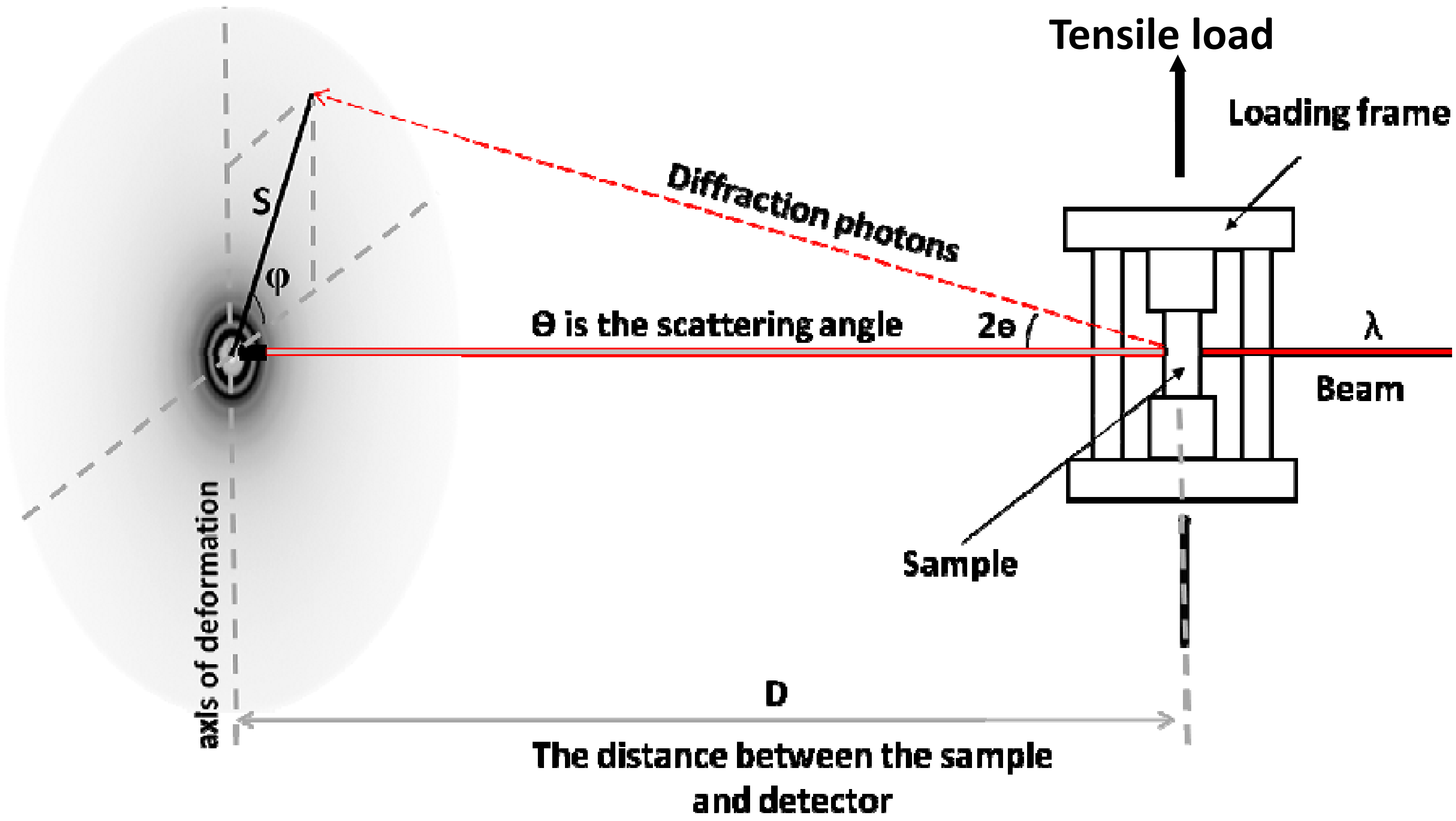




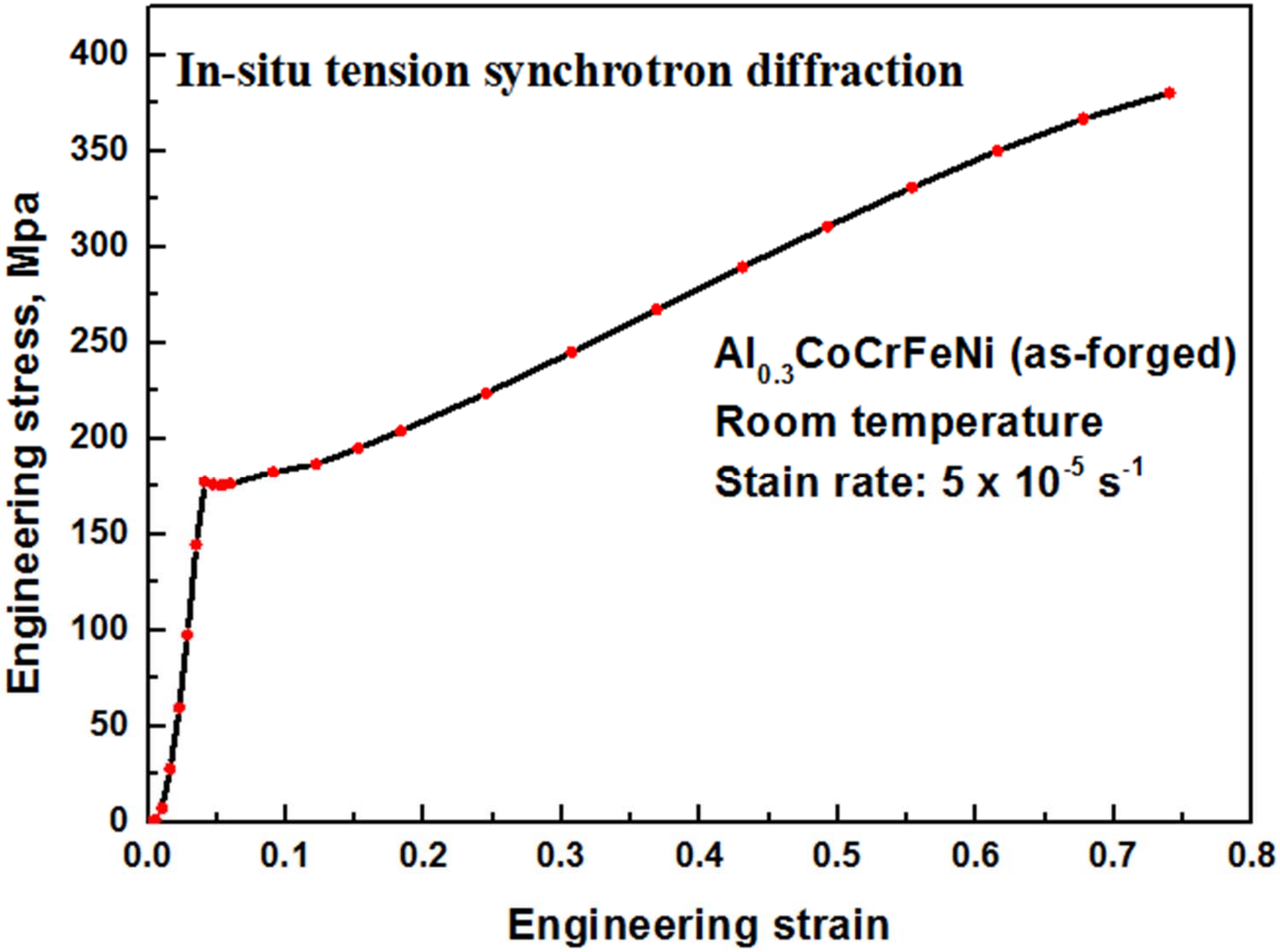
$Al_{0.3}$CoCrFeNi-as-HIPed (Room Temperature)

- ➢ The neutron-pair-distribution-function (PDF) data and the calculated PDF agree well at larger distances.
- ➢ As shown by the difference curve, the agreement for the second peak is worse.
- ➢ This trend is consistent with the expectation that single-phase HEAs are still locally strained, and yet, possess long-range crystal order.

In-situ Synchrotron Results

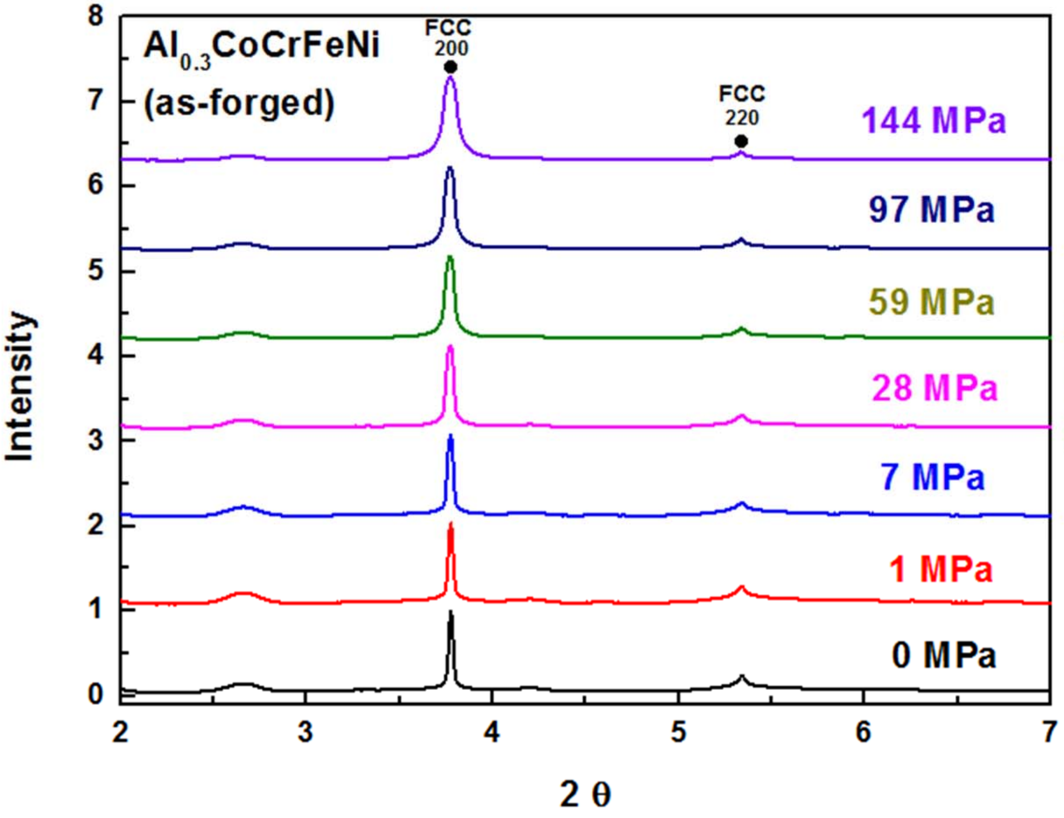


In-situ Synchrotron Results

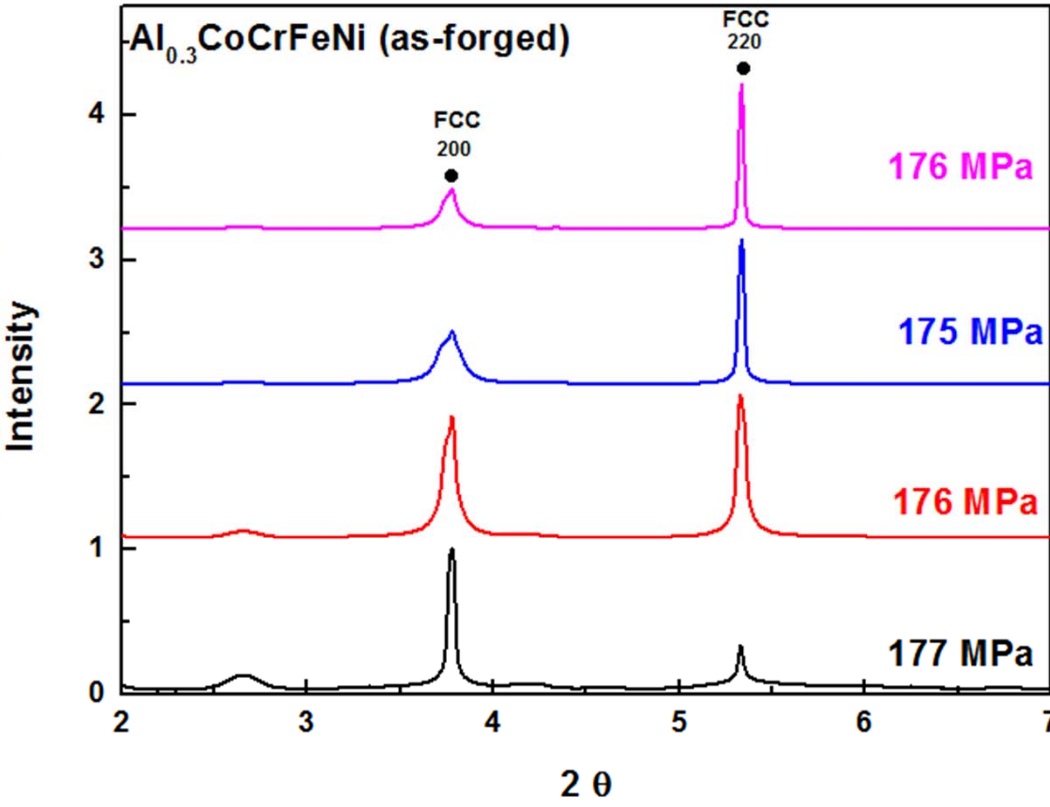


In-situ Synchrotron Results

Elastic region

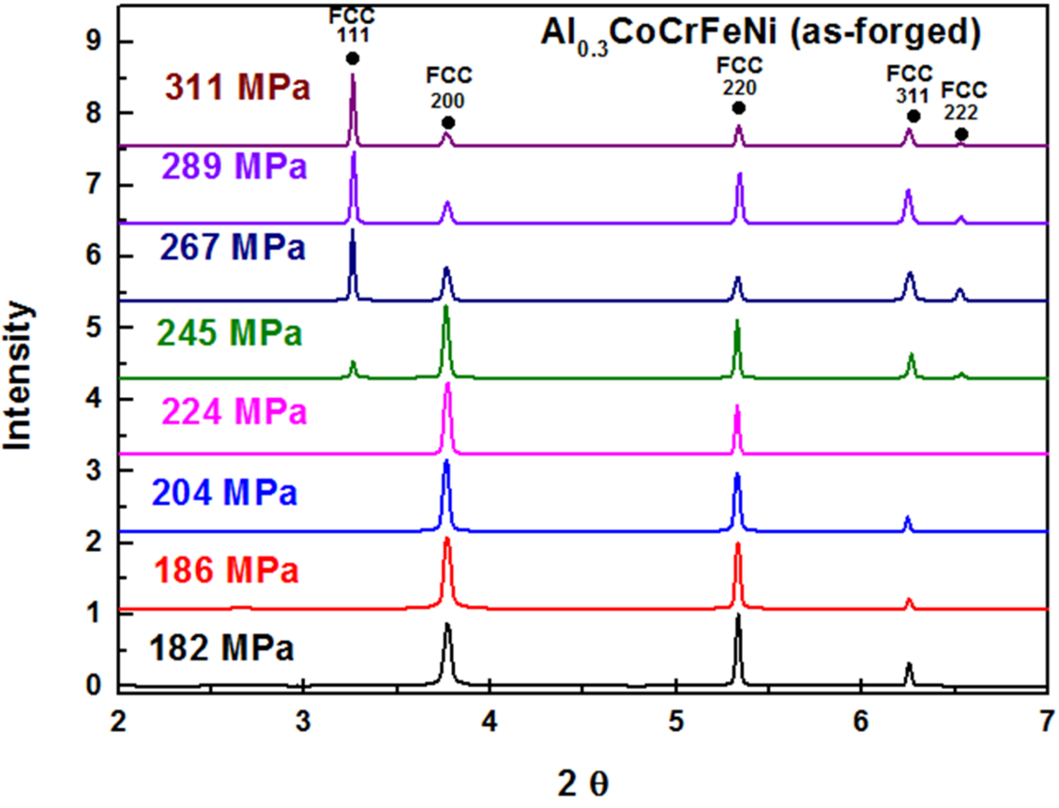


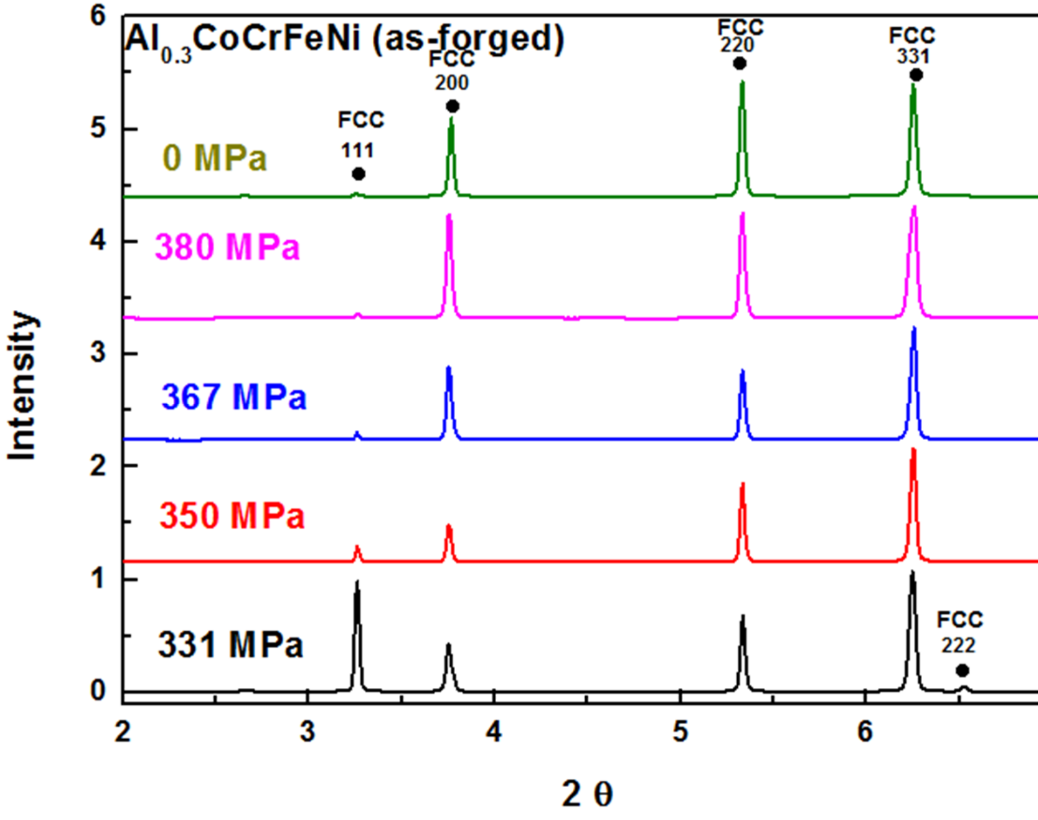
Yielding stage



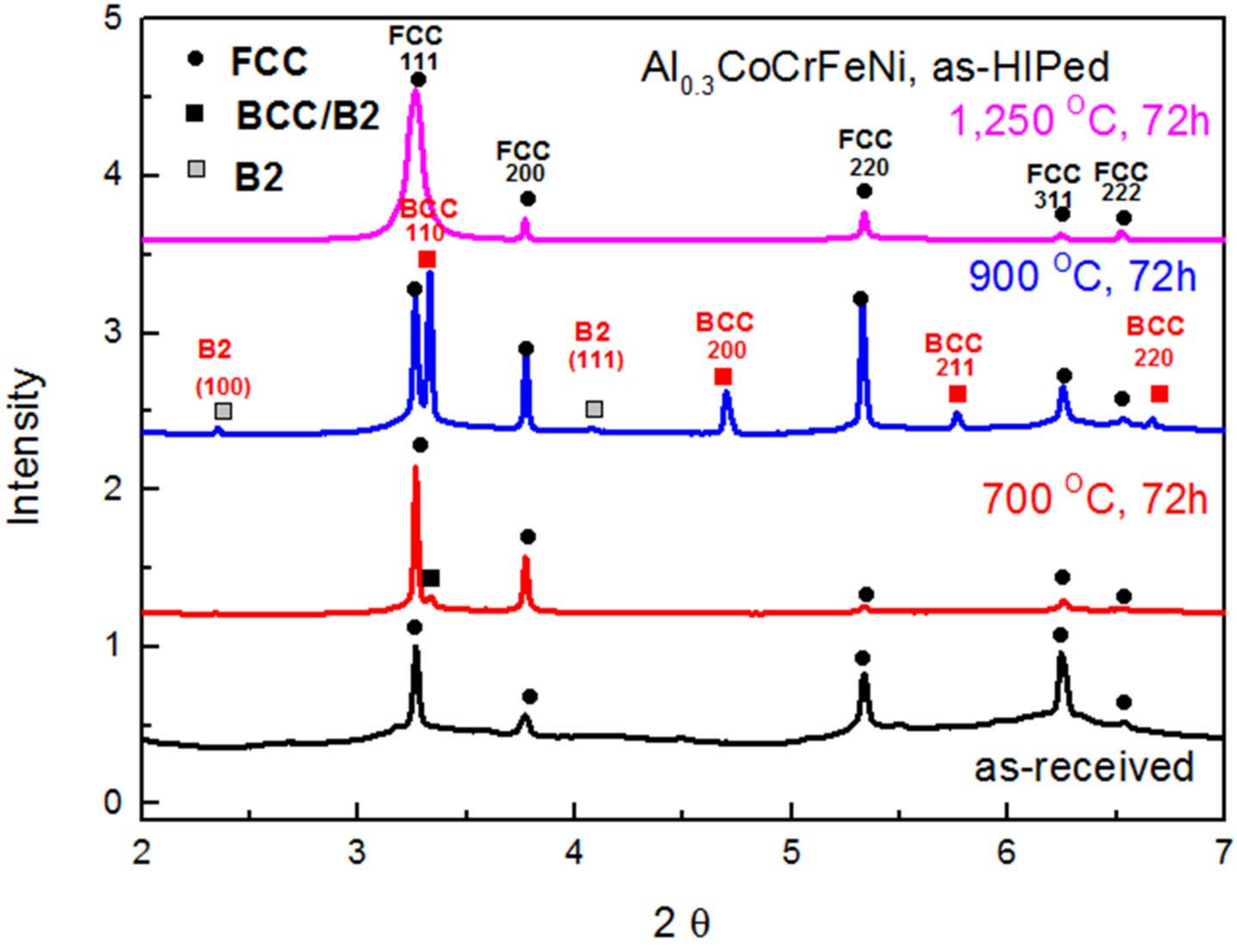
In-situ Synchrotron Results

Plastic region





Heat-treatment effect (Synchrotron X-ray pattern)



- ❑Heat-treated at 1,250 °C for 72 h
  FCC
- ❑Heat-treated at 900 °C for 72h,
  FCC + B2
- ❑Heat-treated at 700 °C for 72h,
  FCC + BCC (small)

Conclusions

$Al_{0.3}CoCrFeNi$

- **It is a single-phase FCC HEA**
- **The mechanical behavior is the best among the presently published single-phase FCC HEAs.**
- **Below 550 °C, the mechanical behavior is stable.**
- **At 550 °C and 100 MPa, the creep rate is relatively low.**
- **Following heat treatments at 700 °C and 900 °C, the strengthening second phase appears**