Multi-modal Approach to Modeling Creep Deformation In Ni-Base Superalloys

FE0031554

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DOE-NETL's 2020 Virtual Integrated Project Review Meeting: High Performance Materials

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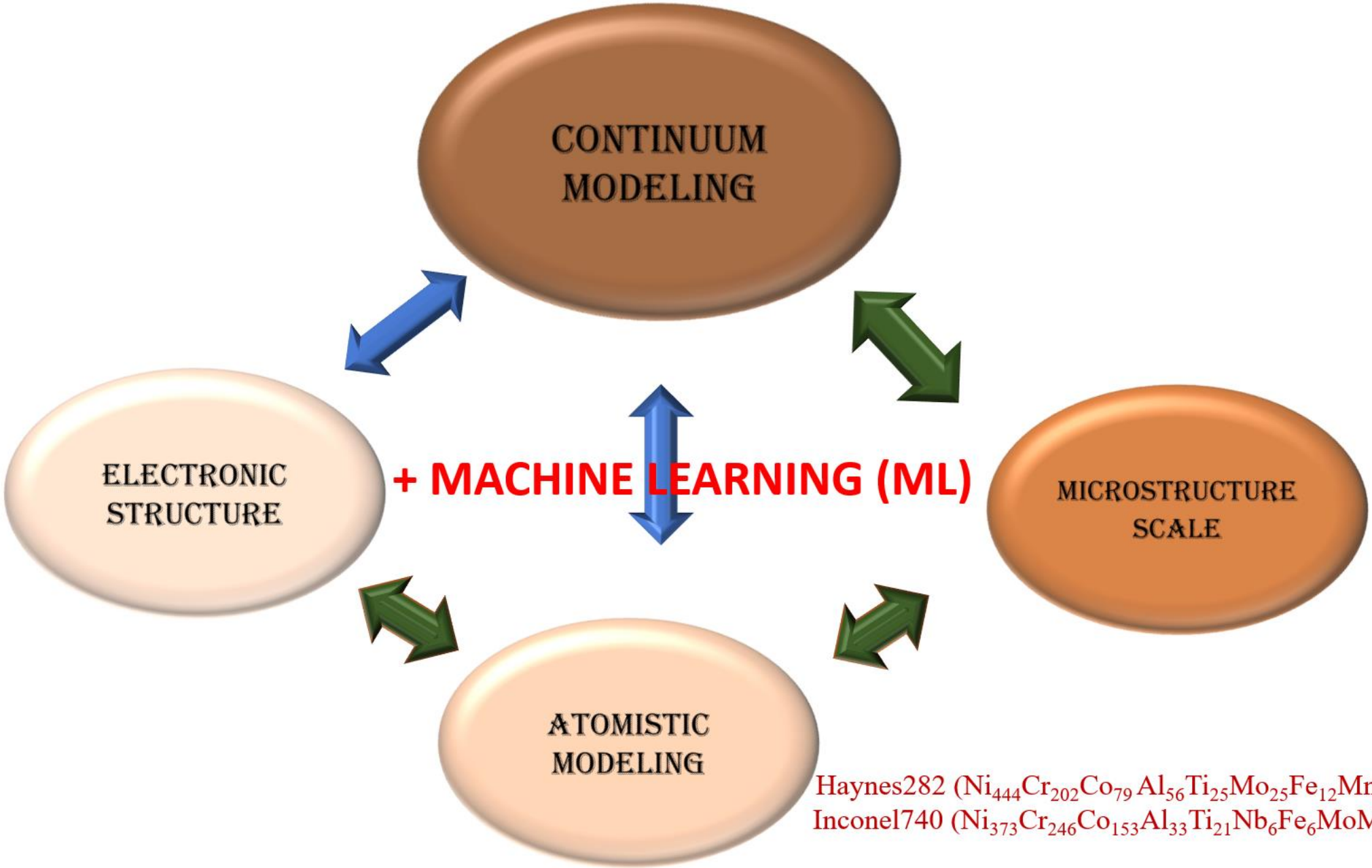
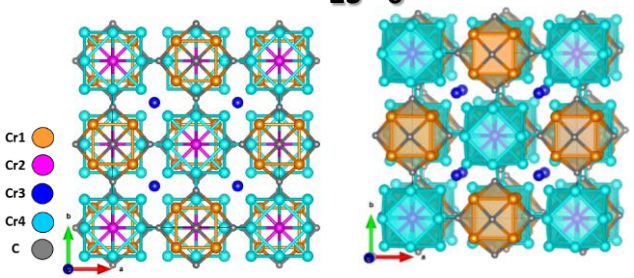


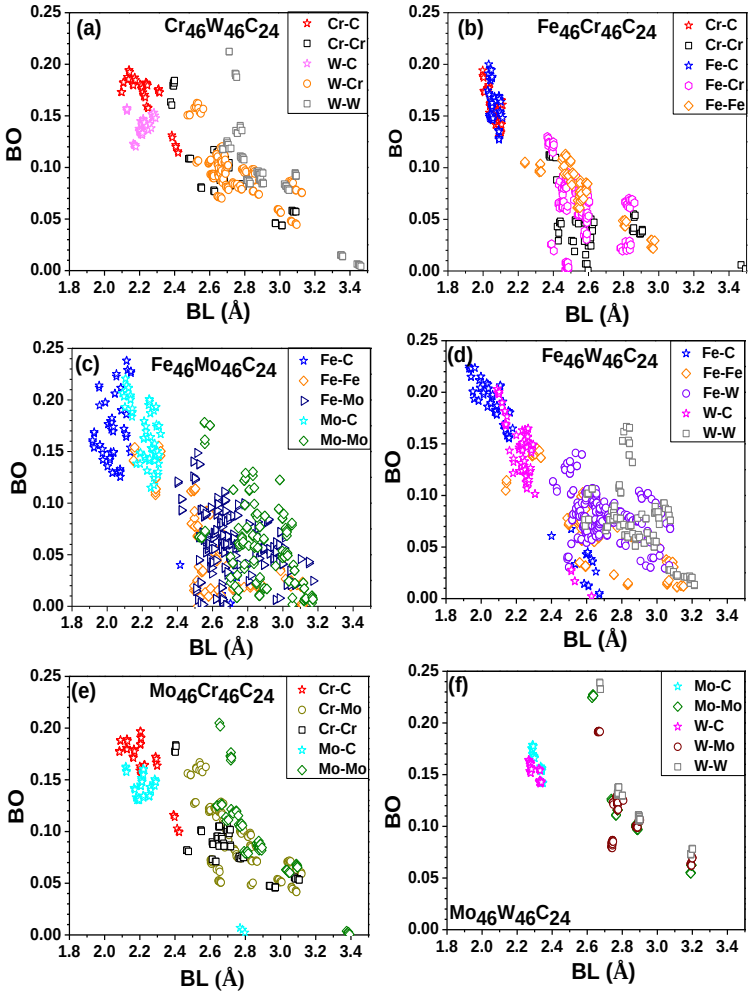
Haynes282 ($Ni_{444}Cr_{202}Co_{79}Al_{56}Ti_{25}Mo_{25}Fe_{12}Mn_3Si_5C_{12}B$)
Inconel740 ($Ni_{373}Cr_{246}Co_{153}Al_{33}Ti_{21}Nb_6Fe_6MoMn_3Si_{17}C_5$)

Electronic Structure-based Modeling:

$M_{23}C_6$



➢ Predicting fundamental material properties



Bond order vs. bond length of ternary carbides

	C11	C12	C44	K	G	E	η	G/K	A^U	H
$Cr_{92}C_{24}$	472.15	211.53	124.88	298.427	126.63	332.82	0.3141	0.4243	0.0098	10.69
$Fe_{92}C_{24}$	432.09	246.42	58.24	308.414	69.65	194.32	0.3950	0.2258	0.3047	3.42
$Mo_{92}C_{24}$	457.24	220.09	113.51	299.138	116.28	308.81	0.3279	0.3887	0.0017	9.11
$W_{92}C_{24}$	510.38	252.59	136.12	338.521	133.14	353.12	0.3261	0.3933	0.0035	10.16
$Cr_{46}W_{46}C_{24}$	474.07	231.08	105.97	312.469	109.47	294.07	0.3431	0.3503	0.1488	7.76
$Fe_{46}Cr_{46}C_{24}$	471.16	221.87	118.87	304.802	122.98	325.19	0.3222	0.4035	0.0099	9.89
$Fe_{46}Mo_{46}C_{24}$	436.32	218.30	88.34	293.452	93.02	252.39	0.3567	0.3170	0.0786	6.17
$Fe_{46}W_{46}C_{24}$	466.93	241.65	92.20	314.966	96.88	263.60	0.3605	0.3076	0.1561	6.14
$Mo_{46}Cr_{46}C_{24}$	435.71	219.83	114.08	293.647	111.48	296.88	0.3315	0.3797	0.0591	8.61
$Mo_{46}W_{46}C_{24}$	482.57	232.39	111.06	317.581	115.47	308.95	0.3379	0.3636	0.0211	8.40

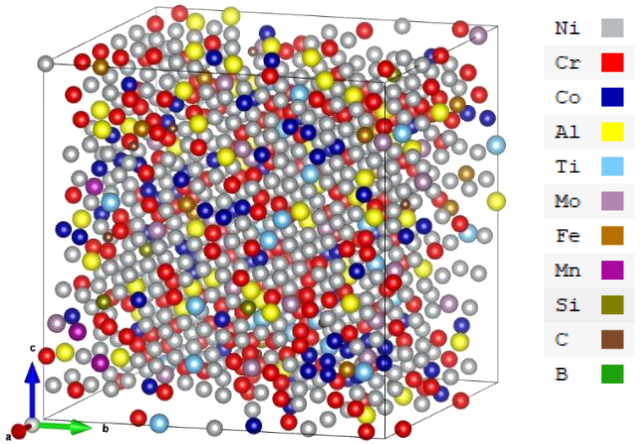
Calculated Cij, Shear modulus (G), bulk modulus (K), Young's modulus (E), Poisson's ratio (η), Pugh's modulus ratio (k = G/K), Universal anisotropy A^U and Vicker's Harness H

Electronic Structure-based Modeling:

- Developing large-scale alloyed models for γ and/or γ' structures

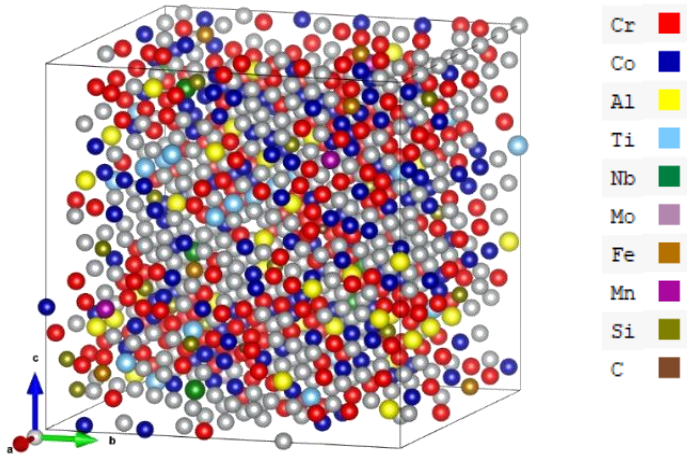
γ

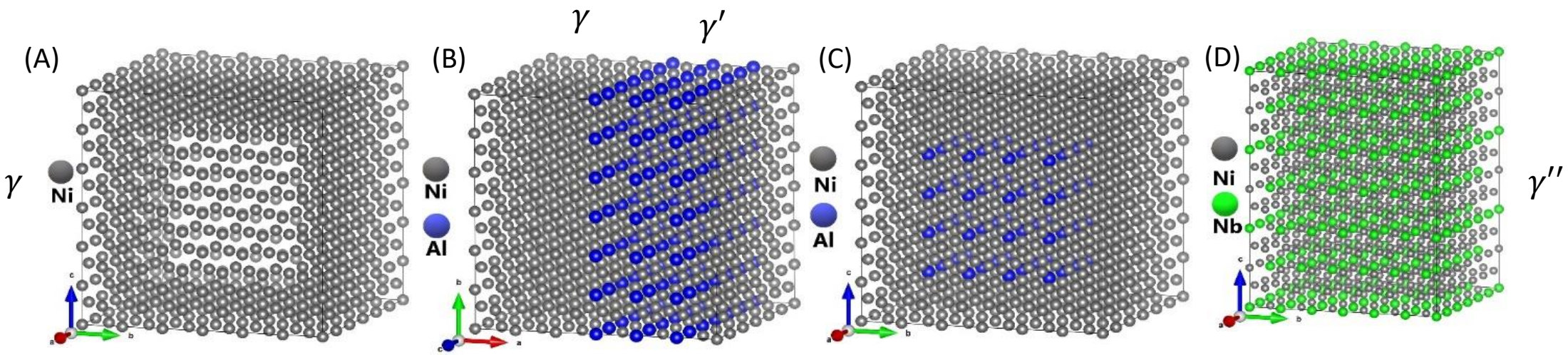
Haynes 282



γ

Inconel 740



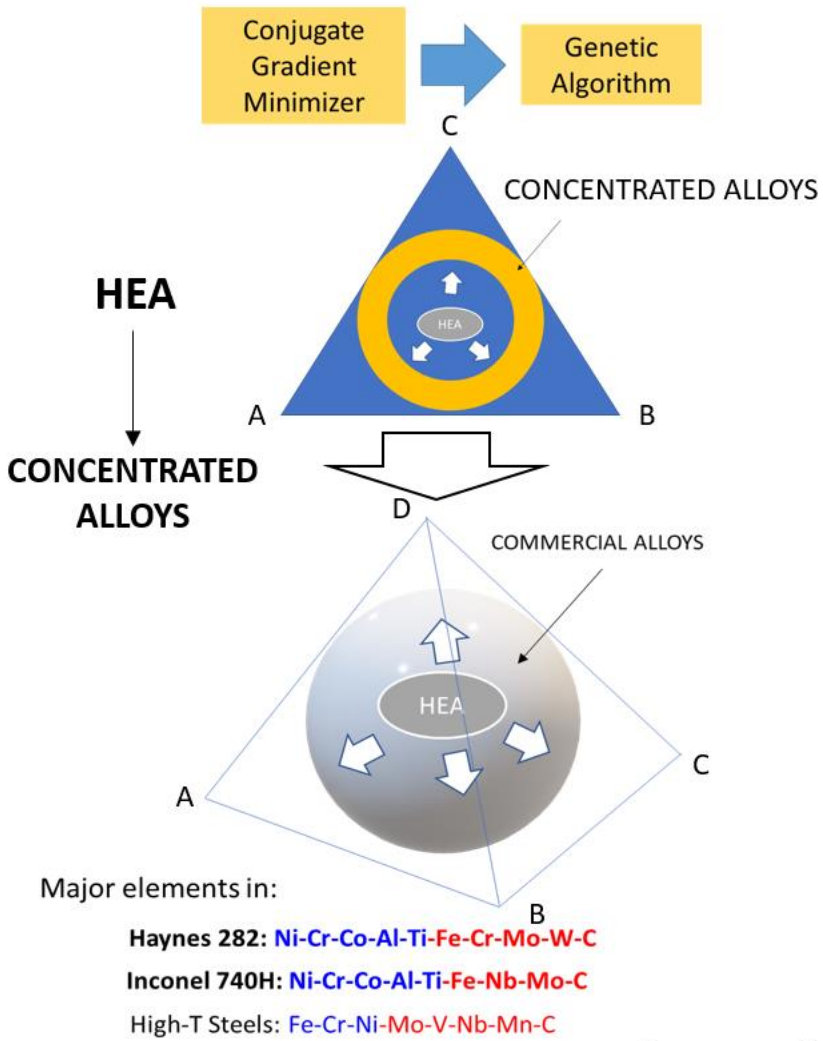


Superalloy models of (A) γ + vacancy (B) γ/γ' interface (C) $\gamma+\gamma'$, and (D) γ'' Ni_3Nb

Atomic-based Modeling:

➢Developing multi-component interatomic-potentials

Energy, Force & Stress Sampling from Electronic Structure Calculations



Major elements in:

Haynes 282: Ni-Cr-Co-Al-Ti-Fe-Cr-Mo-W-C

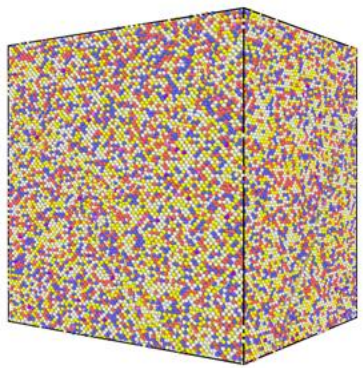
Inconel 740H: Ni-Cr-Co-Al-Ti-Fe-Nb-Mo-C

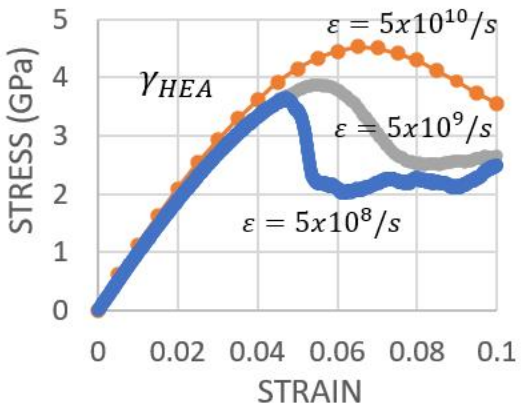
High-T Steels: Fe-Cr-Ni-Mo-V-Nb-Mn-C

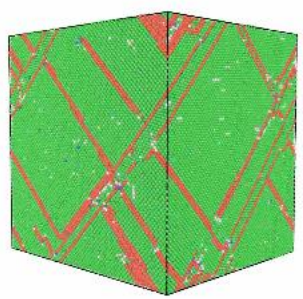
$\gamma + \gamma'$ system

Ni-Co-Cr-Fe-Al, Ni-Co-Cr-Fe-Al-Ti-Nb

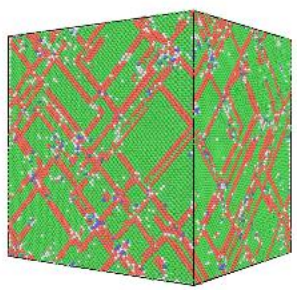
$(Ni_{20}Co_{20}Cr_{20}Fe_{20}Al_{20})_{99}(Ti_{50}Nb_{50})_1$







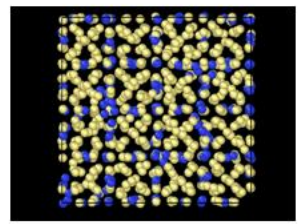
Strain Rate = $5*10^8$



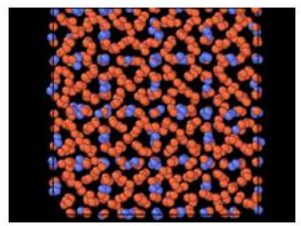
Strain Rate = $5*10^9$

Carbide system

Fe-C, Cr-C, Mo-C, W-C and Mo-C



$Cr_{23}C_6$ 2000K



$W_{23}C_6$ 3000K

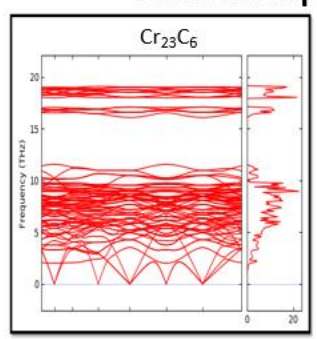
Elastic Constants

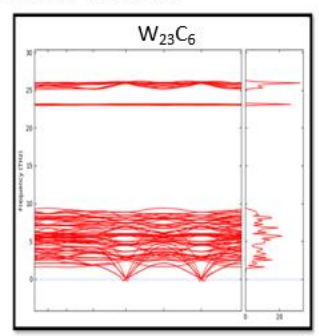
Elastic Constants	EAM (GPa)	DFT* (GPa)
Bulk	286	298
Shear Modulus	121	126
Poisson	0.366	0.314
C11	398	472
C12	230	211
C44	121	125

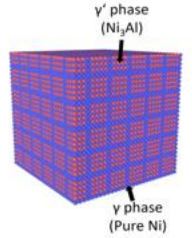
Elastic Constants	MEAM (GPa)	DFT* (GPa)
Bulk	399.516	338.521
Shear Modulus	137.288	133.14
Poisson	0.383	0.3261
C11	535.034	510.38
C12	331.758	252.59
C44	137.282	136.12

* Puja Adhikari et. al., Materials Research Express, Vol 6 [11], 116323, (2019)

Phonon Dispersion Curves



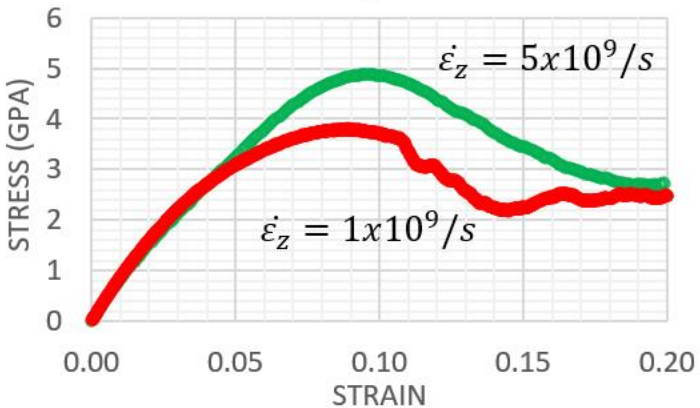


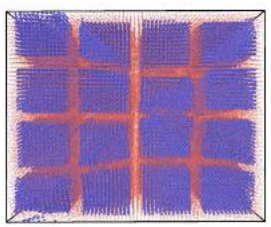


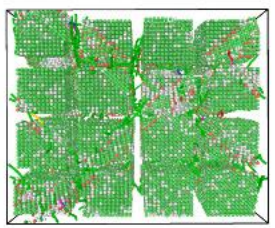
Atomic-based Modeling:

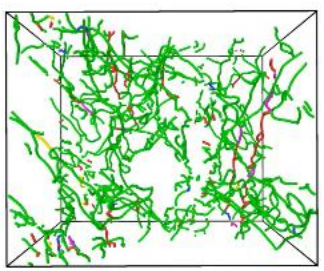
➢ Modeling deformation using MD simulations aided by Machine Learning

Simulated compression tests



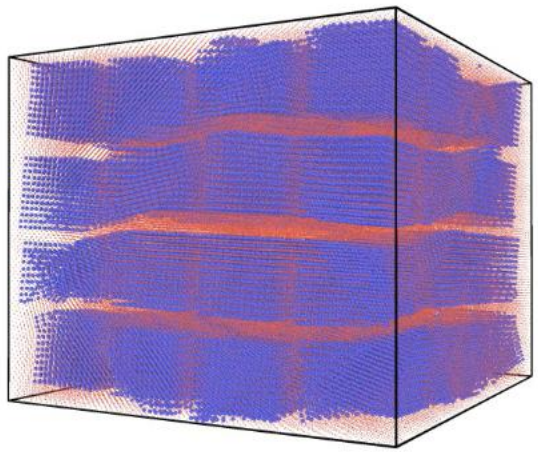






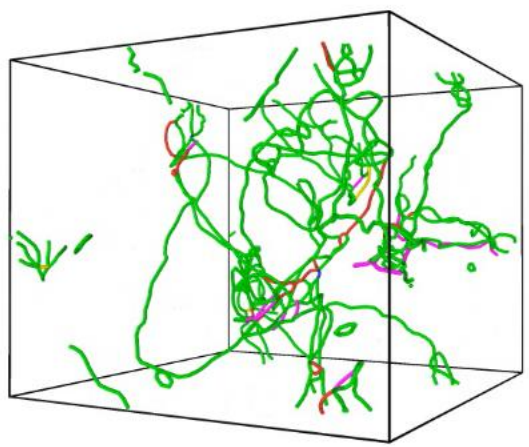
$\dot{\varepsilon}_z = 1x10^9/s$

Simulated creep tests

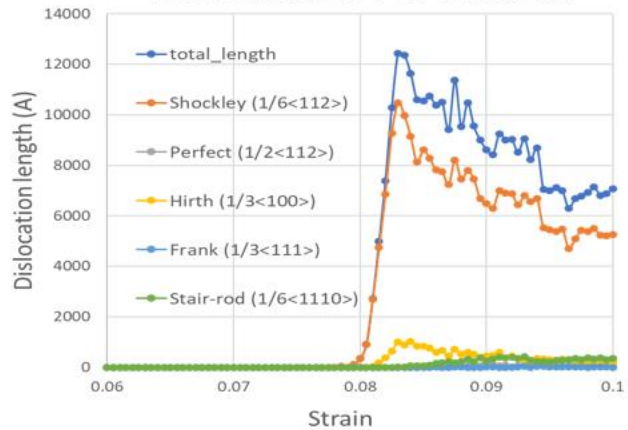


1000K

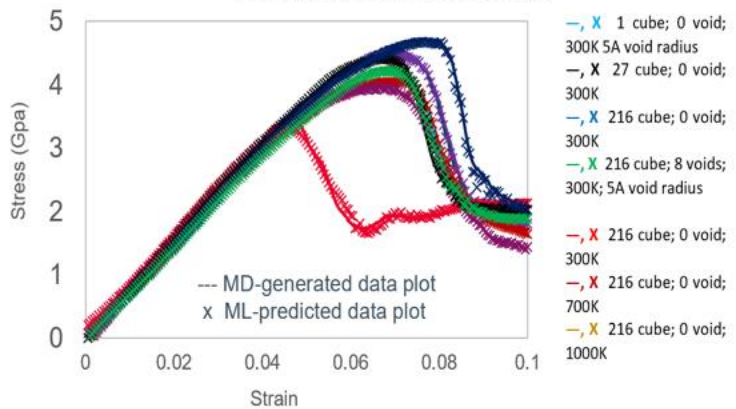
$\sigma_z = 2.0 - 4.0\ GPa$



DISLOCATION POPULATION



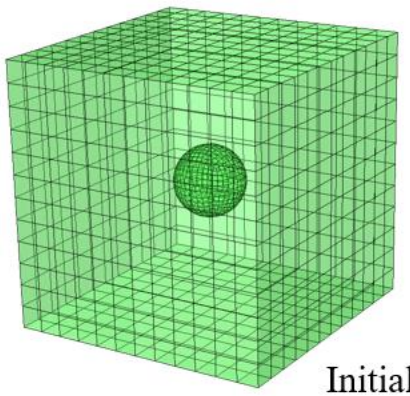
MACHINE LEARNING

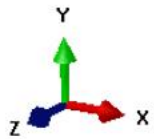


Continuum-based modeling

➢Developing crystal plasticity models

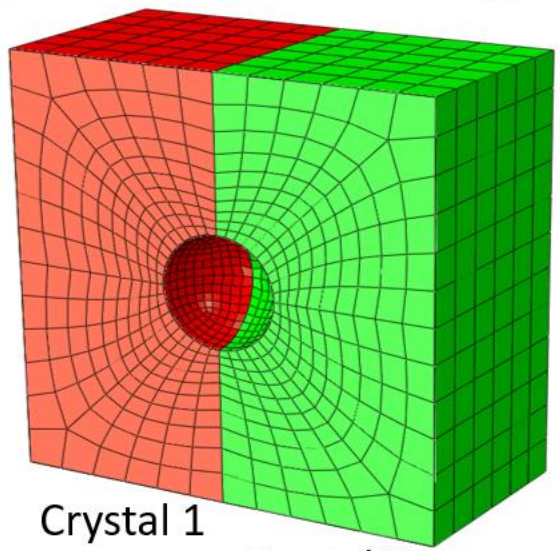
Finite element mesh for void growth





6128 elements

Initial void volume fraction, $f_0 = 0.01$

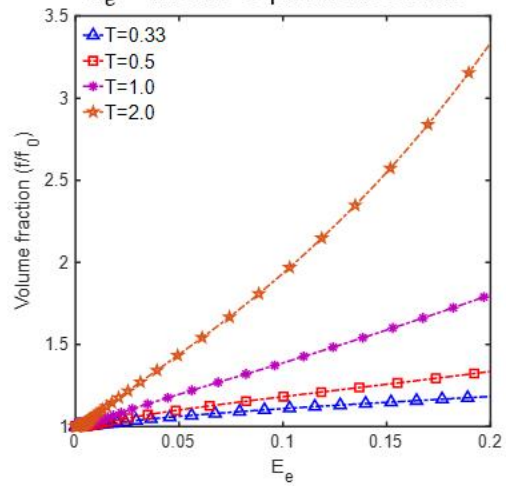


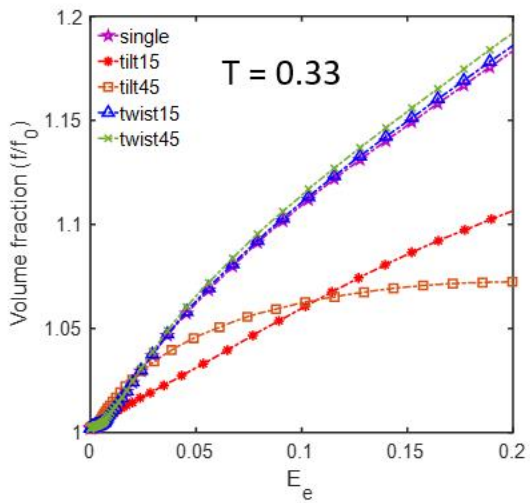
Crystal 1

Crystal 2

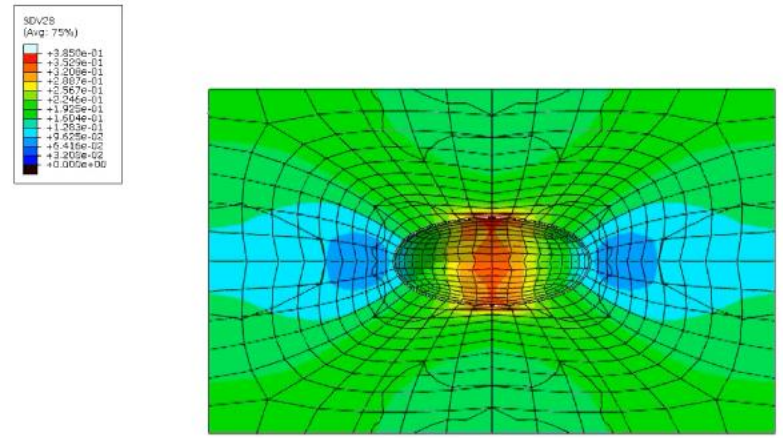
T (stress triaxiality)= $\frac{\sum h}{\sum e}$

E_e =macro-equivalent strain



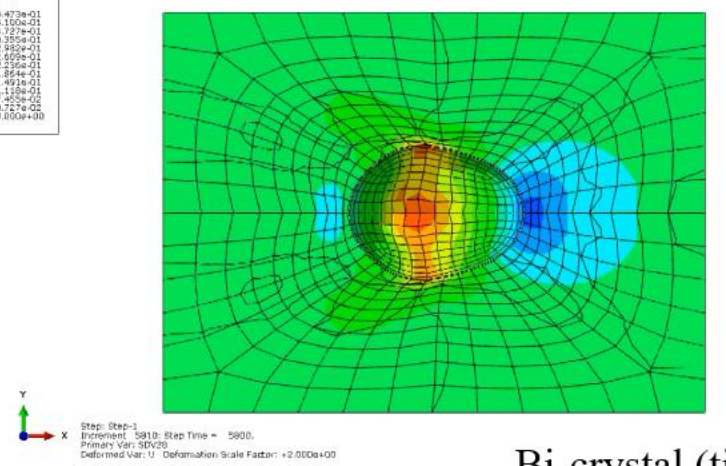


Distribution of plastic strain around deformed voids



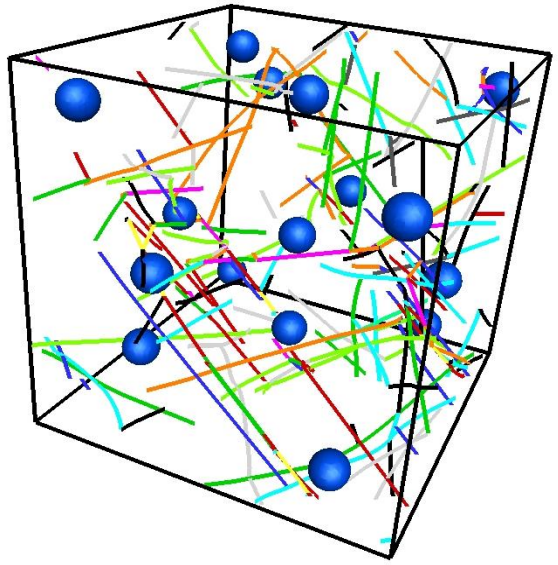
Single Crystal

T = 0.33



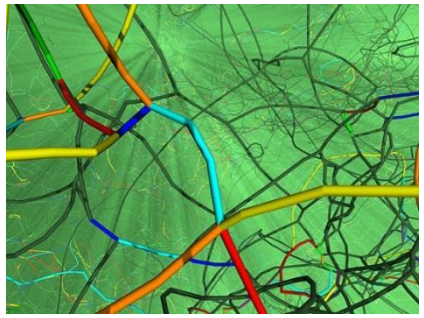
Bi-crystal (tilt 45°)

➢ Strengthening mechanisms in Ni-based Superalloys



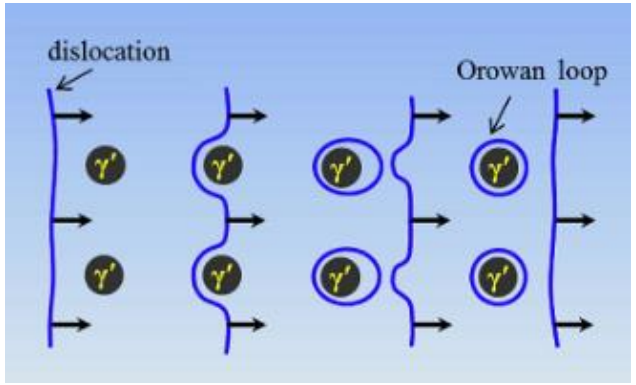
Development of Continuum-based models

Dislocation interaction

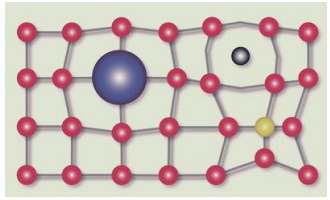


Materials science and technology 25.2 (2009): 213-220.

Dislocation looping

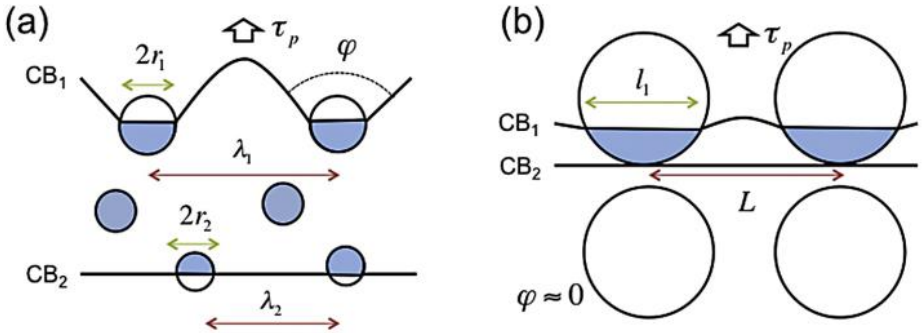


Journal of Alloys and Compounds 687 (2016): 389-401



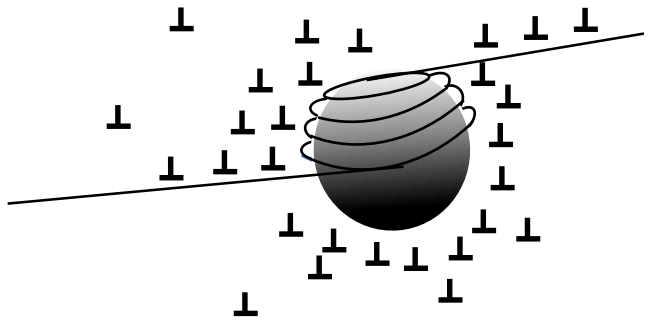
Solid solution

Dislocation shearing



Acta Materialia 98 (2015): 377–390

Multi-modal modeling dislocation climb for creep deformation

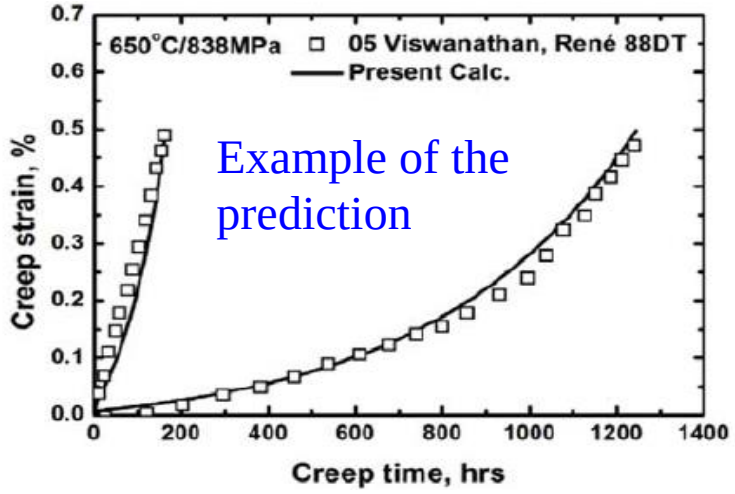


- During the high temperature and low stress creep region, the rate of dislocation climb controls the dislocation velocity.
- The shear strain rate on each slip system is expressed as

$$\dot{\gamma}^{\alpha}_{climb} = \rho^{\alpha}_{m} f_p \frac{\lambda_{eff}}{r_p} c_{jog} D_s * \sinh\left[\frac{(\tau^{\alpha} - \tau_{resistance}) b^2 \lambda_{eff}}{k_B T}\right] * sign(\tau^{\alpha})$$

where ρ^{α}_{m} is mobile dislocation density on α slip system , f_p is the volume fraction of the γ′ phase, λ_{eff} is the effective dislocation moving distance and r_p is the average particle radius. c_{jog} is the dislocation line jog density, D_s is the bulk diffusivity. $\tau_{resistance}$ comes from the interactions of dislocations with solutes, partials and other dislocations.

- Lower length-scale i.e. electronic structure (ES), MC & MD calculations can provide the following information for calculation of the shear strain rate:
  - **Antiphase boundary & SF energy (ES, MC & MD)**
  - **Temperature-dependent modulus (ES & MD)**
  - **Particle shear strength (ES & MD)**
  - **Diffusivity (MD)**



International Journal of Plasticity 110 (2018) 123-144

Presentations and publications

Presentations (underlined: undergraduate students):

- (Invited) Ridwan Sakidja and Wai-Yim Ching, "Compositional Design and Deformation Behavior in Ni-based Concentrated/HEA Alloys“, TMS Annual Meeting & Exhibition, Sun, Feb 23, 2020 – Thu, Feb 27, 2020, San Diego, CA.
- (Invited) Caizhi Zhou, Tianju Chen, Ridwan Sakidja, Wai-Yim Ching, "Effect of the crystallographic orientation on the void growth during creep of superalloys", TMS 2019 Annual Meeting & Exhibition, March 10-14, 2019, San Antonio, Texas.
- Puja Adhikari, Saro San, CiaZhi Zhou, Rdiwan Sakidja, and Wai-Yim Ching, *First-principles calculation of crystalline precipitate phases $M_{23}C_6$(M = Cr, W, Mo, Fe) in Ni-based supper-alloys, XVI European Ceramic Conference in Torino (Italy) June16-20, 2019.*
- Wai-Yim Ching and Saro San, Electronic structure and mechanical properties of Ni-based superalloys: Haynes282 and Inconel740, 43rd ICACC, Jan 27-Feb-1 2019, Daytona Beach, FL.
- Saro San and Wai-Yim Ching, Ab initio modeling of large defects in -Ni and -Ni, 43rd ICACC, Jan 27-Feb-1 2019, Daytona Beach, FL.
- Austin Bollinger, Ridwan Sakidja, "Molecular Dynamic Simulations of Layered Metallic Systems". Presentations at the Arkansas Idea Networks of Biomedical Research Excellence (INBRE), Nov. 2nd-3rd,2018 at the University of Arkansas in Fayetteville, AR.
- Tyler McGilvry-James, Nirmal Baishnab, Ridwan Sakidja, "Molecular Dynamics (MD) Potential Development for Carbides". Presentations at the Arkansas Idea Networks of Biomedical Research Excellence (INBRE), Nov. 2nd-3rd,2018 at the University of Arkansas in Fayetteville, AR.
- Rabbani Muztoba, Nirmal Baishnab, Sabila Kader, Ridwan Sakidja– Development of multi-component EAM potential for Ni-based Superalloys, Presentations at the Materials Science & Technology (MS&T)2018 in Columbus, OH , October 14-18, 2018
- Sabila Kader Pinky, Muztoba Rabbani, Ridwan Sakidja –Molecular Dynamics Study of Creep Deformation in Nickel-based Superalloys, Presentations at the Materials Science & Technology (MS&T)2018 in Columbus, OH , October 14-18, 2018

Theses:

- Tianju Chen, PhD. Thesis: Mechanical behavior of metallic composites with using crystal plasticity method, Missouri University of Science & Technology (2020)
- Sabila Kader Pinky, Master’s Thesis: Molecular Dynamics Study of Creep Deformation in Nickel-based Superalloy, Missouri State University, (2019) https://bearworks.missouristate.edu/theses/3461/
- Muztoba Rabbani, Master’s Thesis: Development Of Multicomponenet EAM Potential For Ni-Based Superalloy, Missouri State University, (2019) https://bearworks.missouristate.edu/theses/3460/

Journal publications

- Tianju Chen, Ridwan Sakidja, Wai-Yim Ching, Caizhi Zhou, "Crystal Plasticity Modeling of Void Growth on Grain Boundaries in Ni-Based Superalloys", JOM, Volume 71, Issue 11, pp 3859–3868, (2019).
- Puja Adhikari, Saro San, Caizhi Zhou, Ridwan Sakidja, Wai-Yim Ching, "Electronic structure and mechanical properties of crystalline precipitate phases M23C6 (M = Cr, W, Mo, Fe) in Ni-based superalloys", Materials Research Express, Vol 6 [11], 116323, (2019).
- Wai-Yim Ching, Saro San, Jamieson Brechtl, Ridwan Sakidja, Miqin Zhang, and Peter Liaw, "Fundamental electronic structure and multiatomic bonding in thirteen biocompatible high-entropy alloys", npj Computational Materials, volume 6, Article number: 45 (2020). *-partly supported by this project.*

Summary

Continued development of:

- Fundamental materials properties of alloyed carbide phases.
- Atomistic-based large-scale models for γ and γ+γ’ structures
- Interatomic potentials for multi-component γ + γ’ and binary carbide systems.
- Atomistic-based simulations on the deformation behaviors in alloyed γ + γ’ systems at elevated temperatures.
- Continuum-based crystal plasticity modeling on γ matrix – single crystal & bi-crystal structures.

Tasks to complete in Q4_YR20 & YR21:

- Bond strength analysis at the γ / γ' and $\gamma / M_{23}C_6$ interfaces of the Haynes 282 & Inconel 740.
- Further verifications on the interatomic potentials for $\gamma + \gamma'$system.
- Development on transferable interatomic potentials for the multi-component carbide system and $\gamma + \gamma'$plus carbide system.
- Extracting temperature-dependent and creep-related materials database from electronic structure and MD simulations.
- Integrate the results and database from lower scale models into crystal plasticity-based creep models for Haynes 282 and Inconel 740.

Extra slides

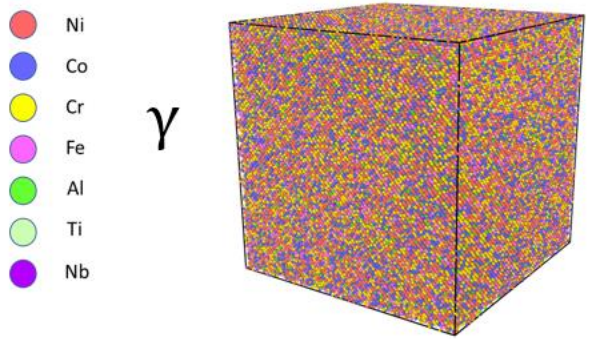
Multi-modal Approach to Modeling Creep Deformation In Ni-Base Superalloys

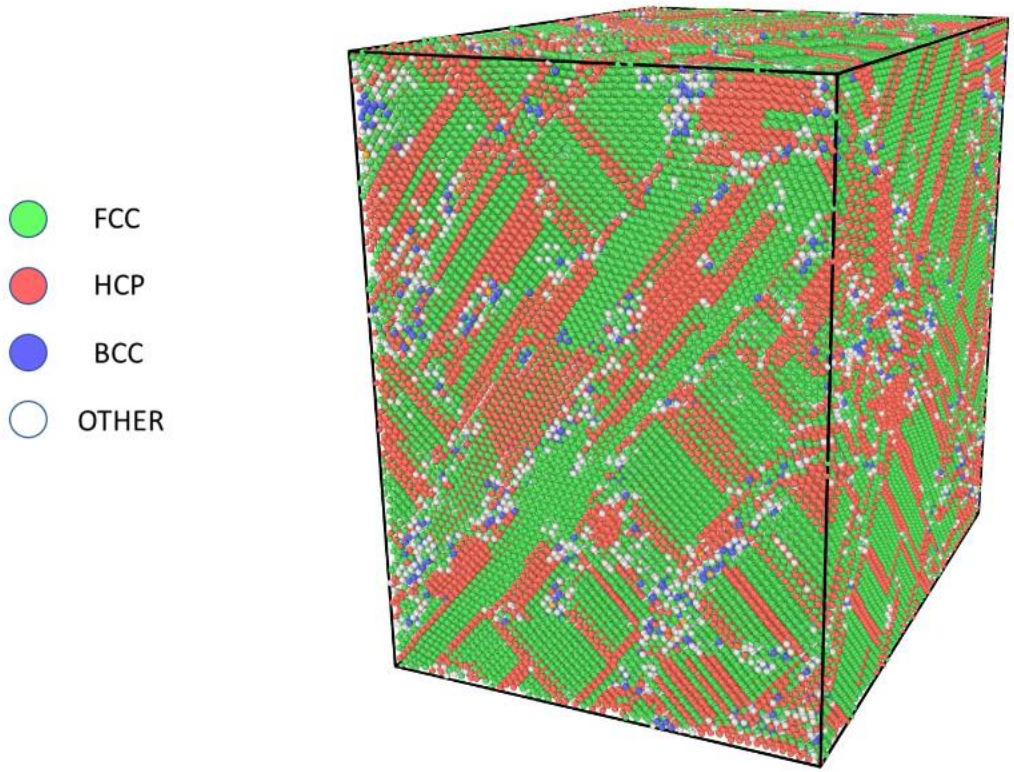
HEA-GGP

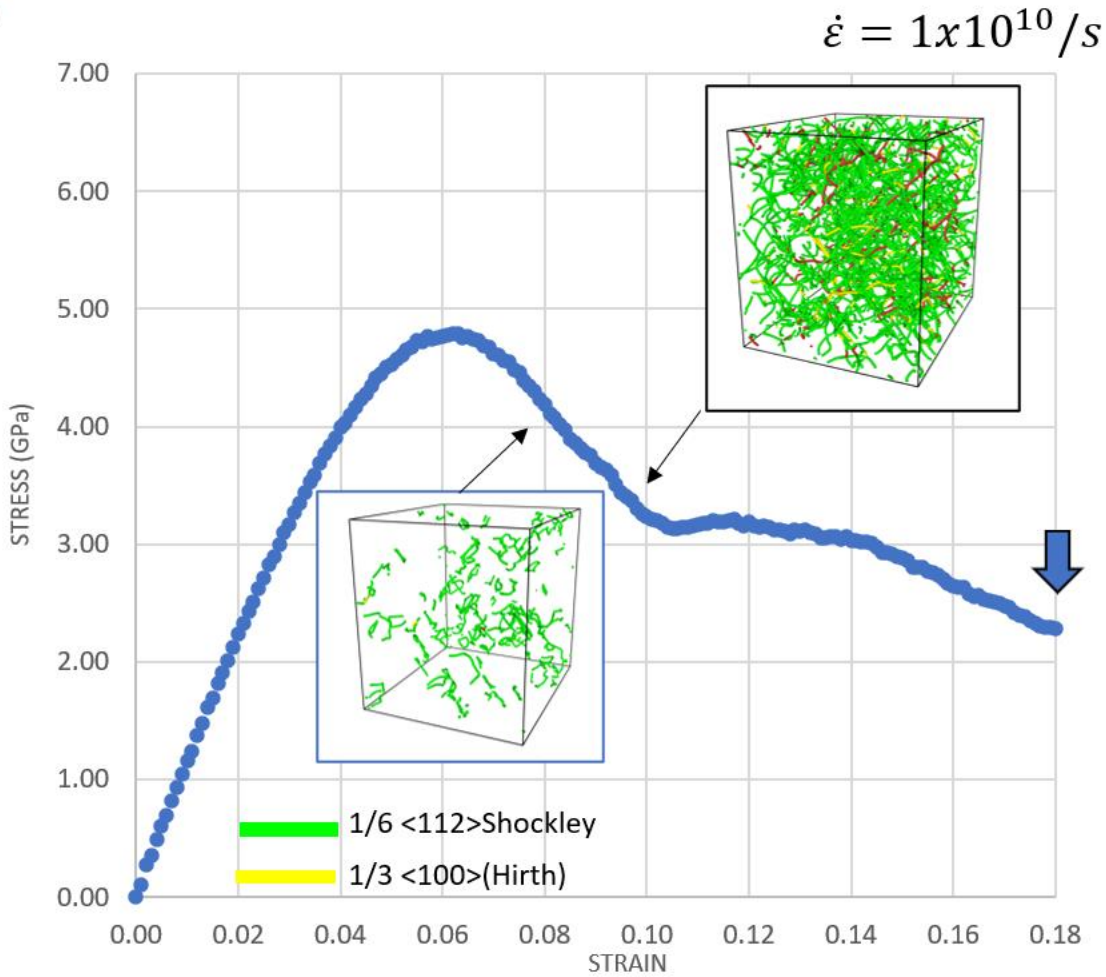
Ni-Co-Cr-Fe-Al-Ti-Nb

HEA EAM POTENTIAL: COMPOSITION & STABILITY TEST

300K

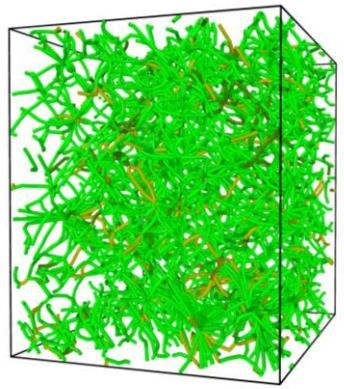






Multi-modal Approach to Modeling Creep Deformation In Ni-Base Superalloys

γ'

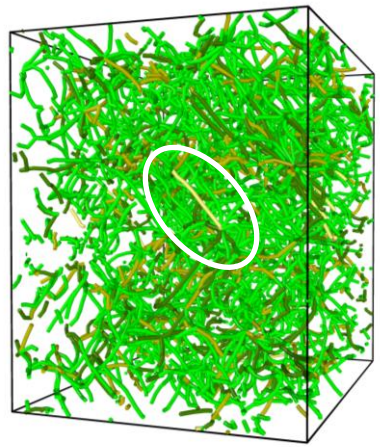


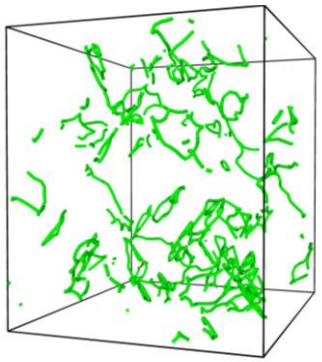
HEA-GGP

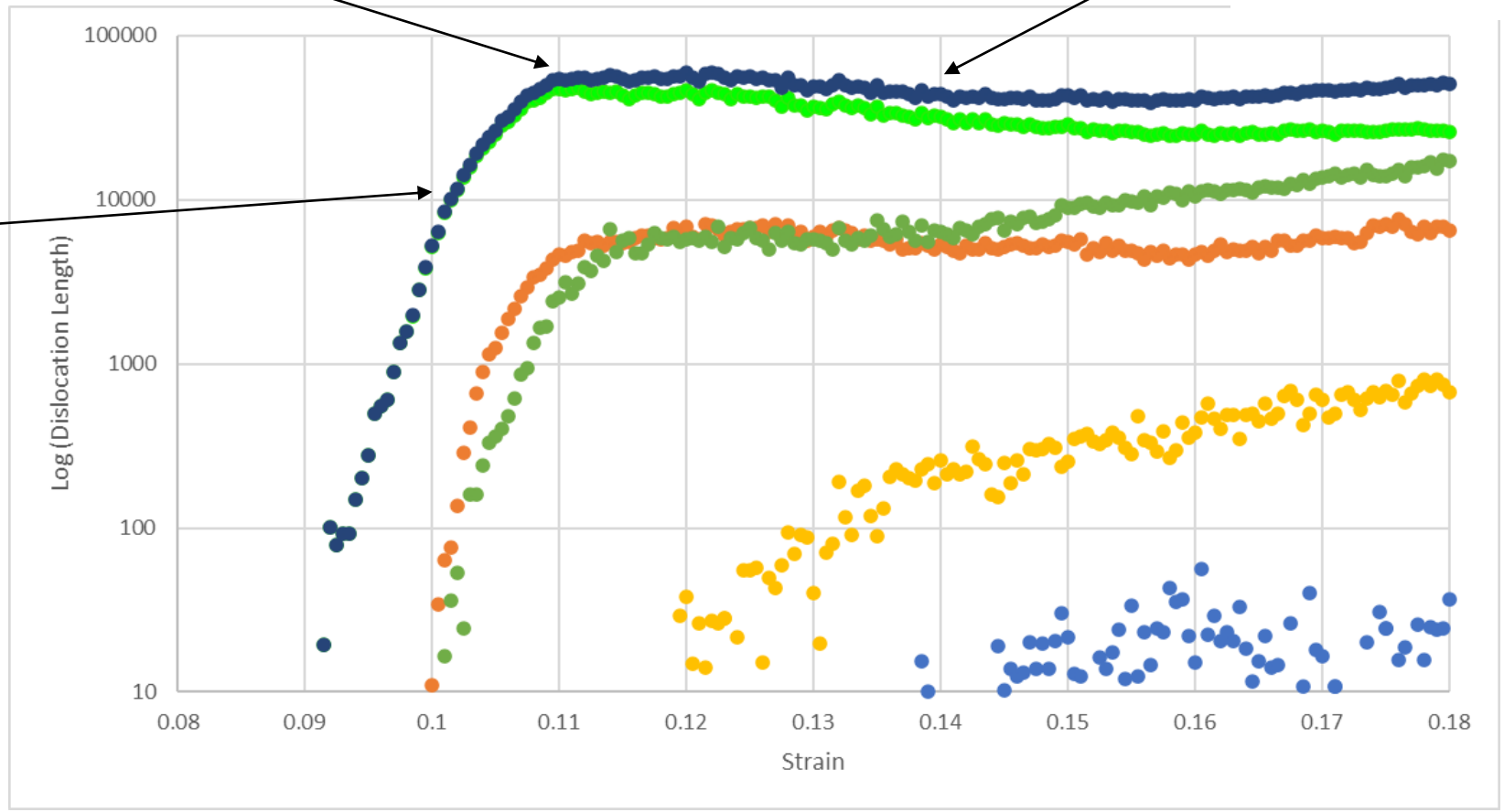
Ni-Co-Cr-Fe-Al-Ti-Nb

HEA EAM POTENTIAL: COMPOSITION & STABILITY TEST

300K







$\dot{\varepsilon} = 1x10^{10}/s$