Multimodal Approach to Modeling Creep Deformation in Ni-base Superalloys

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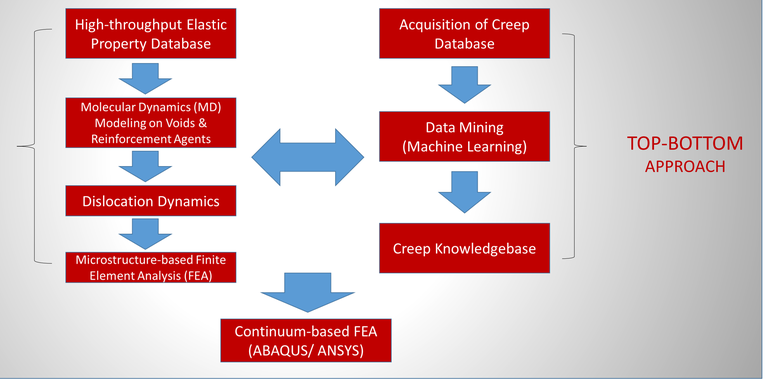
Overall Goals

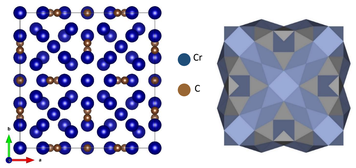
- The overarching goal of the project's approach is to establish a new framework with the adaptation of data mining tools using a rigorous step-by-step atomistic-mesoscale-continuum based simulation.
- This approach will reduce the level of uncertainty of experimental creep data and facilitate a better linkage between the experimentally-acquired creep data and the creep models.
- Ultimately, it will help to improve the quantitative predictive capability for the onset of creep failure during the tertiary creep stage.
- The approach can also be applied to a wider range of material candidates for fossil energy power plants.
- Focus areas: Ni-Al and Ni-Co-Al Base Models, Haynes 282 and Inconel 740 Superalloys

Two-pronged Multi-scale Strategy

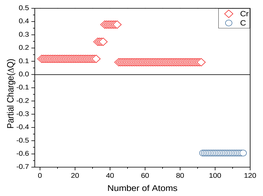


Electronic Structure Calculations

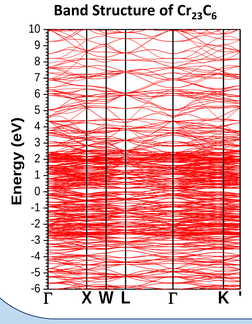
Name: $Cr_{23}C_6$
Lattice parameter:
a = 10.52Å
γ = 90.00°
Space Group: 225
Number of Atom: 116
Types: 5
cell volume = 1165.36 Å³



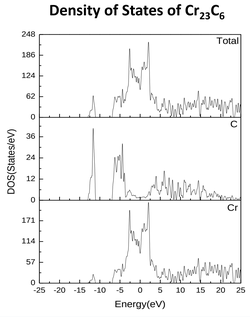
Partial Charges of $Cr_{23}C_6$



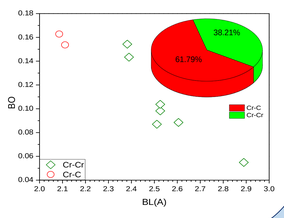
Band Structure of $Cr_{23}C_6$



Density of States of $Cr_{23}C_6$



Bond Order vs. Bond Length of $Cr_{23}C_6$

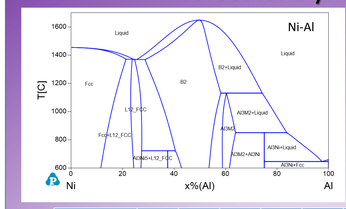


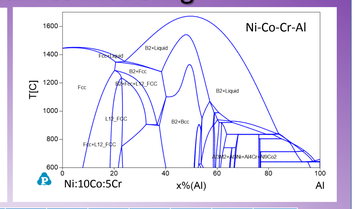
Elastic properties of $M_{23}C_6$

	C11	C12	C44	K	G	E	η	G/K	A^U
$Cr_{92}C_{24}$	472.155	211.529	124.879	298.427	126.634	332.825	0.3141	0.4243	0.0098
$Mo_{92}C_{24}$	457.238	220.087	113.508	299.138	116.275	308.814	0.3279	0.3887	0.0017
$W_{92}C_{24}$	510.384	252.593	136.120	338.521	133.139	353.122	0.3261	0.3933	0.0035
$Fe_{92}C_{24}$	432.089	246.418	58.237	308.414	69.651	194.324	0.3950	0.2258	0.3047

$W_{32}C_6$ exhibits the strongest overall elastic properties

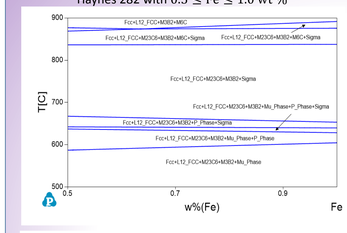
Thermodynamic Database and Molecular Dynamics Modeling



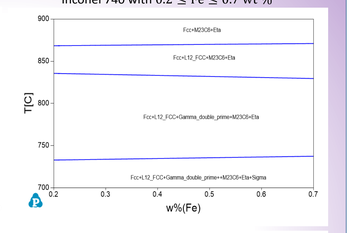


(in at %)	Ni	Cr	Co	Al	Ti	Nb	Mo	Fe	Mn	Si	C	B
Haynes 282	54.8	22.13	9.76	3.2	2.52	0.0	5.1	1.37	0.31	0.31	0.29	0.03
Inconel 740	46.24	27.03	19.08	1.88	2.11	1.21	0.29	0.7	0.31	1.0	0.14	0

Haynes 282 with $0.5 \leq Fe \leq 1.0$ wt %

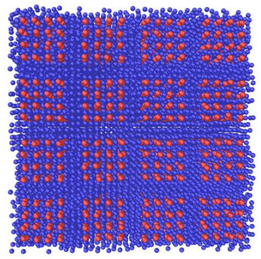


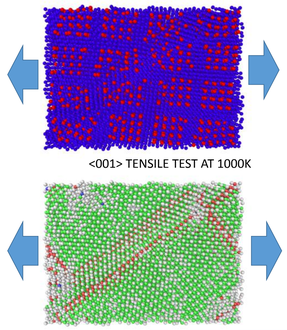
Inconel 740 with $0.2 \leq Fe \leq 0.7$ wt %



MD Modeling on Gamma + Gamma Prime

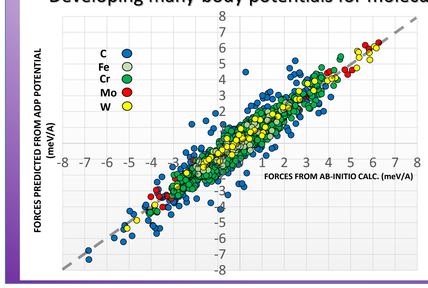
Base Model Ni-Al





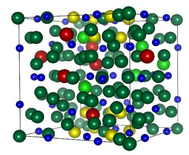
NPT SIMULATIONS AT 1000 K

Developing many-body potentials for molecular dynamics modeling



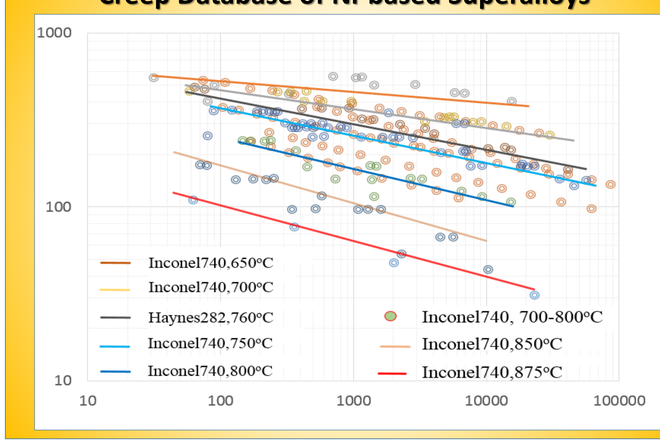
Angular Dependent Potential (ADP)

$$E_{total} = \frac{1}{2}\sum_{i,j(j\neq i)}^{N}\Phi_{ij}(r_{ij}) + \sum_i F(n_i) + \frac{1}{2}\sum_{i,\alpha}(\mu_i^{\alpha})^2 + \frac{1}{2}\sum_{i,\alpha,\beta}\left(\lambda_i^{\alpha\beta}\right)^2 - \frac{1}{6}\sum_i(\nu_i)^2$$

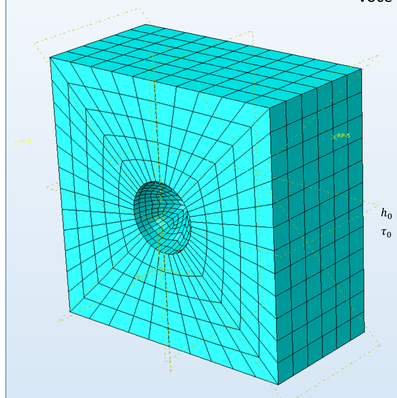


$M_{23}C_6$

Creep Database of Ni-based Superalloys



Crystal Plasticity Simulation of Void Growth



Voce-hardening law : $\dot{\tau}_c^{\alpha} = \sum_{\beta} h_{\alpha\beta}\,|\dot{\gamma}^{(\beta)}|$

$$h_{\alpha\beta} = q_{\alpha\beta} * h$$

$h_{\alpha\beta}$ = strain hardening modulus due to self and latent hardening
$q_{\alpha\beta}$ = interaction coefficients that represent the effect of the hardening between different slip systems
h = self hardening modulus

$$h(\gamma_{\alpha}) = h_s + \left[h_0 - h_s + \frac{h_0 h_s \gamma_{\alpha}}{\tau_s - \tau_0}\right] exp\ -\frac{h_0\gamma_{\alpha}}{\tau_s - \tau_0}$$

h_0 = initial hardening modulus h_s = saturation hardening modulus at large strains
τ_0 = initial yield shear stress τ_s = saturation yields shear stress

$$\gamma_{\alpha} = \int_0^t \sum_{\alpha} |\dot{\gamma}^{(\alpha)}|\,dt$$

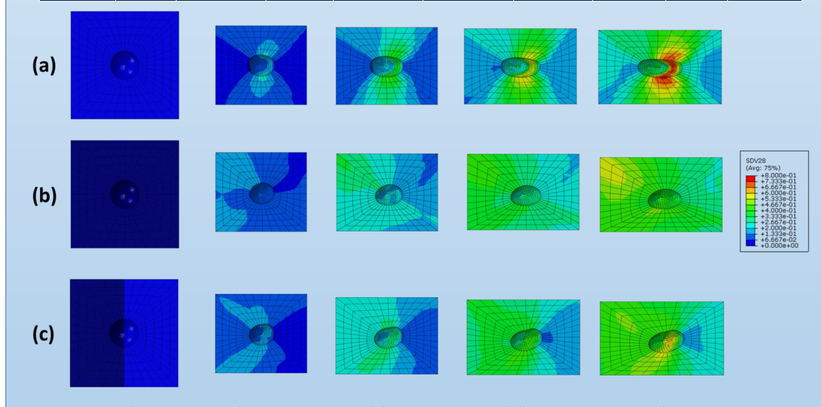
γ_{α} = accumulated shear strain in all slip systems

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left(\frac{|\tau^{\alpha}|}{\tau_c^{\alpha}}\right)^{\frac{1}{m}} sgn(\tau^{\alpha})$$

$\dot{\gamma}^{\alpha}$ = shear strain rate in slip system α

Abaqus CAE: The mesh type is C3D8R, and with total element of 1428. The diameter of the void is D/L=0.2673, leading to an initial void volume fraction f=0.01. The strain rate is $\dot{\gamma} = 1 \times 10^{-3} s^{-1}$ and the total strain is 0.2 along positive, respectively. The boundary condition is that, the z+ surface is set U3=0, and the center of the void is set U1, U2 and U3 all equal to 0.

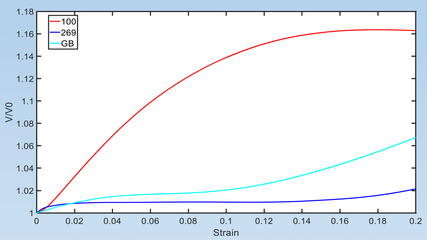
C_{11}	C_{12}	C_{44}	τ_0	τ_s	h_0	h_s	m	$q_{\alpha\beta}$	$\dot{\gamma}$
259.6 GPa	179 GPa	109.6 GPa	465.5	598.5 Mpa	6.0 GPa	0.3 Gpa	1	0.017	0.00242



The initial and deformed mesh for the void growth in (a) the single crystal orientating in [100] direction, (b) the single crystal orientating in [269] direction, (c) grain boundary between [100] and [269] grains.

$$V = \frac{4}{3} * \pi * a * b * c$$

The void in [100] orientated single crystal grew fastest among the three cases, while in the [269] orientated single crystal grew slowest. The void on GB grew relative slow and was affected more by the [269] grain.



The evolution of the volume of the void with the applied strain.

Summary

We have started the initial implementation of the multi-modal approach:

Collection of creep data to be used in data mining tools
Electronic structure & elastic properties of critical precipitatets
Molecular Dynmaics EAM potential tests
Initial MD simulations on deformation of $\gamma + \gamma'$ structures
Initial development of the plasticity model for void growth in Ni-based polycrystalline Superalloys

Acknowledgement

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Program Manager: Richard J. Dunst