Computational Microstructural Optimization Design Tool for High Temperature Structural Materials

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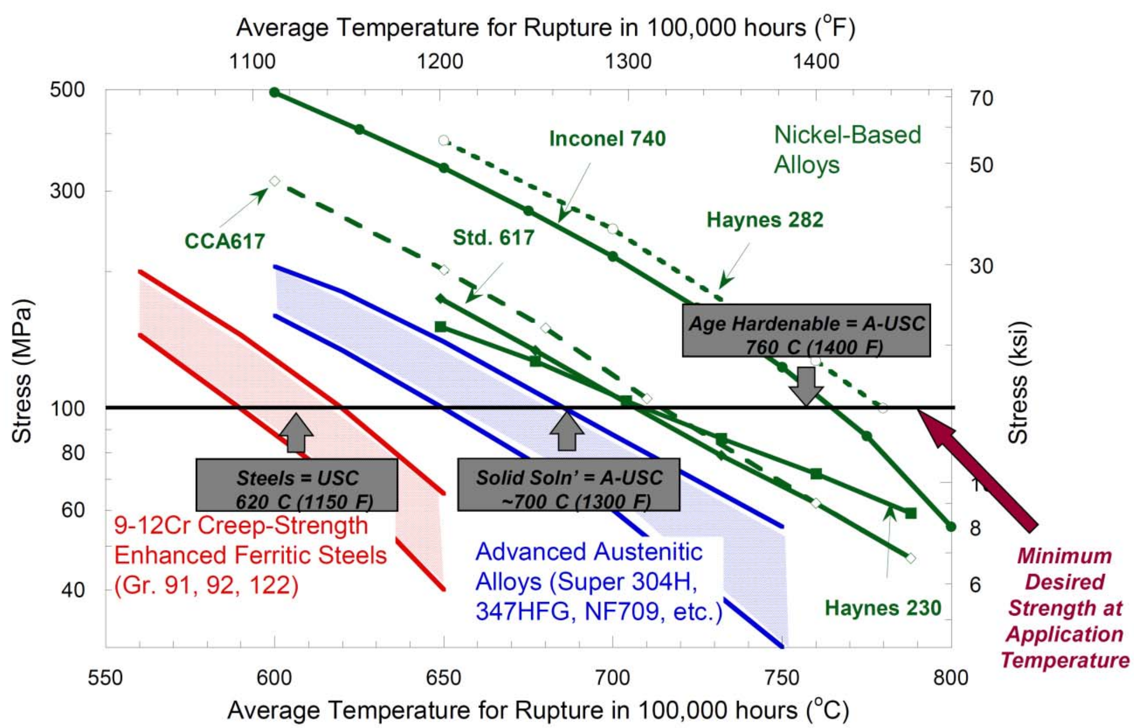
Objectives

- Develop a methodology for microstructural optimization of alloys - genetic algorithm approach for alloy microstructural optimization using theoretical models based on fundamental micro-mechanisms, and
- Develop a new computationally designed Ni-Cr alloy for coal-fired power plant applications.

Robert R. Romanosky, National Energy Technology Laboratory , April 2012

Materials Limit the Current Technology



Background – A Bit of History

Timeline of dislocation-particle strengthening

- Dispersion strengthening identified as a potent mechanism for enhancing elevated temperature strength in the early works of Ansell and Weertman in 1950s
  - CONCEPT- Elastically hard particle repels dislocation
- Srolovitz and co-workers in 1980s
  - FUNDAMENTAL SHIFT- dislocation-particle interaction undergoes repulsive→attractive transition at elevated temperatures >0.35 T_m

Questions

- Why did it take 40 years from the initial papers on dispersion strengthened materials and empirical development of threshold stress for creep to come up with physics based models?
- Why is the development of high temperature alloys incremental and primarily dependent on experiential approaches?

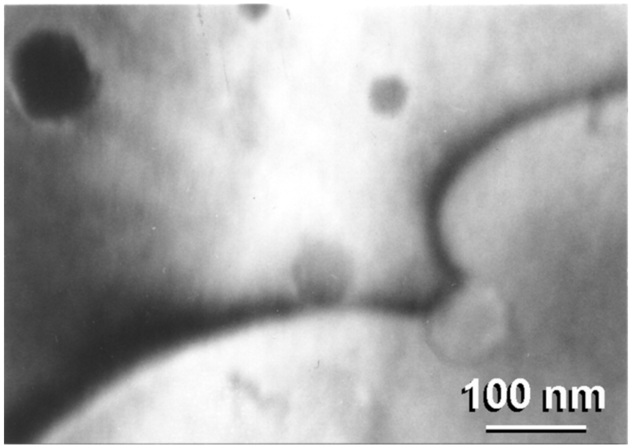
Is it because the field lacks proper computation tools and theoretical development!

Background

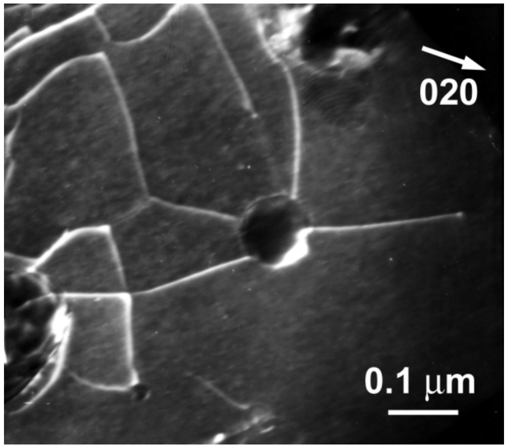
Summary of some of the key development made possible by TEM studies

Reference	Remarks
Nardone and Tien (1993)	First identification of departure side pinning.
Schroder and Arzt (1985)	Weak-beam micrographs showing clear dislocation contrast at the dispersoid.
Herrick et al. (1988)	First quantification of (a) percentage dislocation looped vs. attached, and (b) critical take-off angle as a function of temperature.
Liu and Cowley (1993)	Multiple dislocation-particle interaction; sharp kinks on the detached dislocations that straighten out.

A dispersion strengthened platinum alloy (Heilmaier *et al.* 1999)

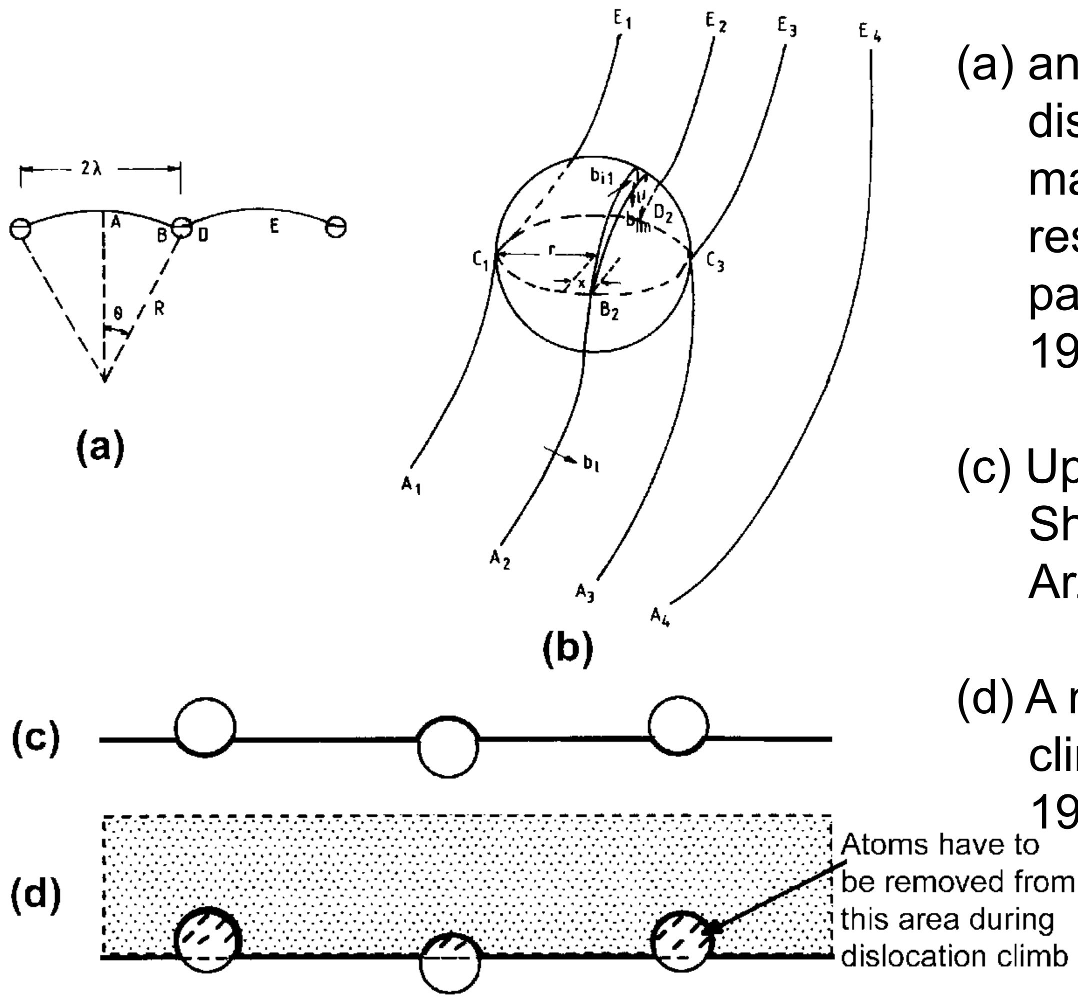


Al-5 wt.% Ti alloy (Mishra and Mukherjee 1995)



Background – Theoretical Models

Development of dissociation and positive climb concepts



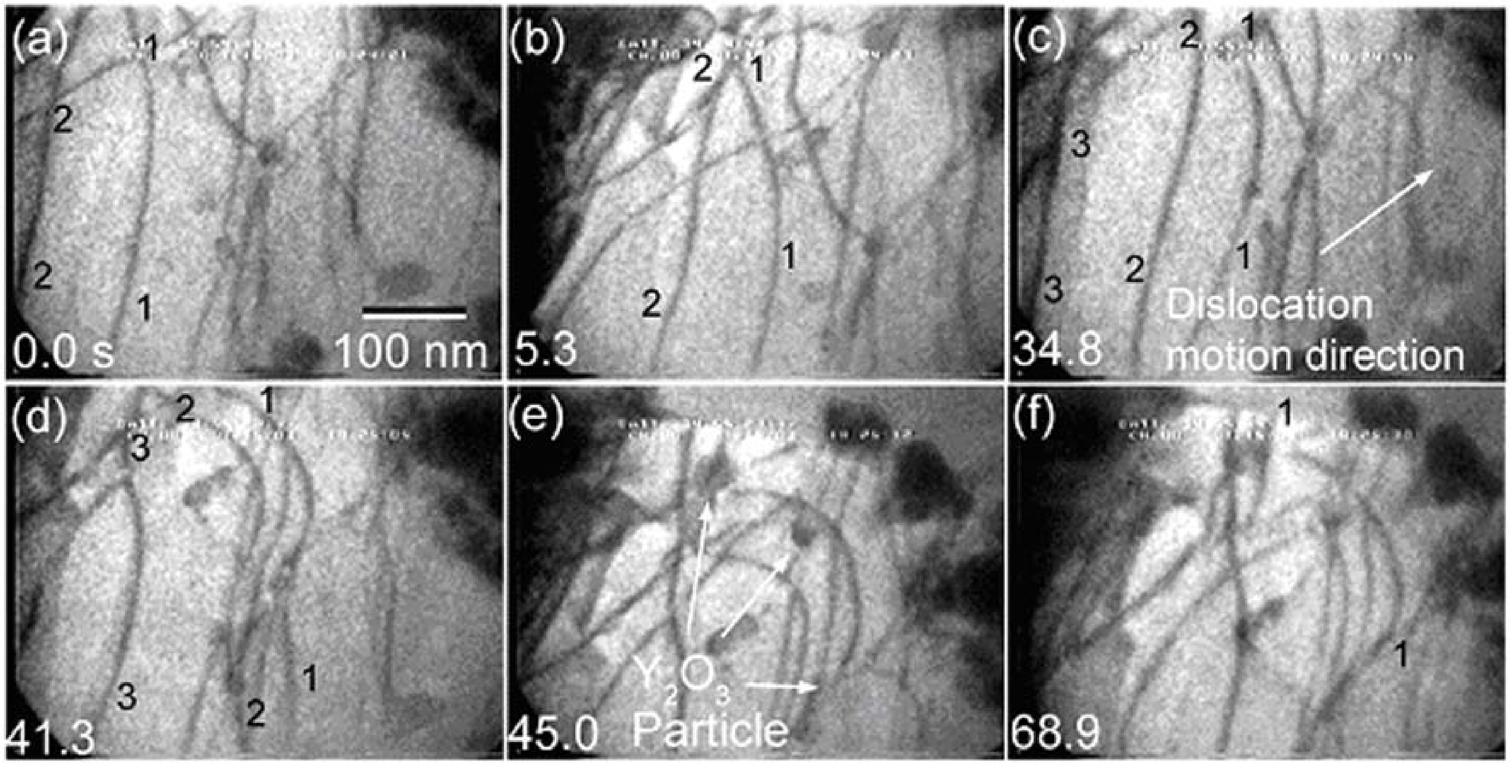
(a) and (b) A schematic illustration of dissociation of dislocation at matrix-particle interface that can result in an attractive dislocation-particle interaction (Mishra et al. 1994).

(c) Up and down climb concept of Shewfelt and Brown (1977) and Arzt and Ashby (1982).

(d) A modified concept of 'positive climb' (Mishra and Mukherjee 1995).

Background – In-situ TEM

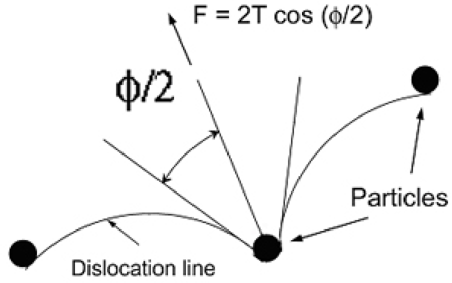
High Temperature In-situ TEM Straining Experiment and Detachment Angle Measurement

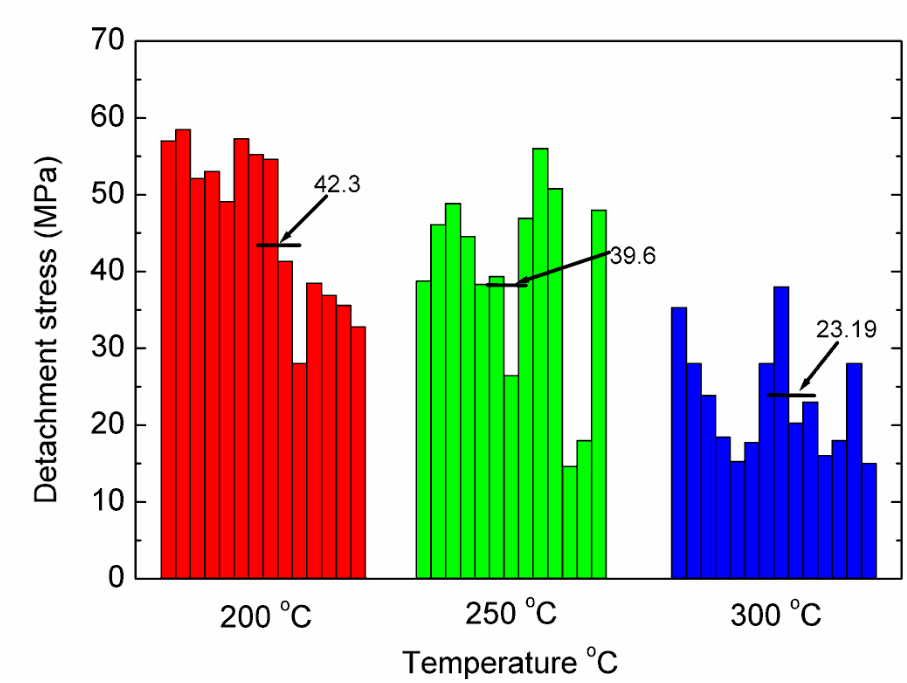


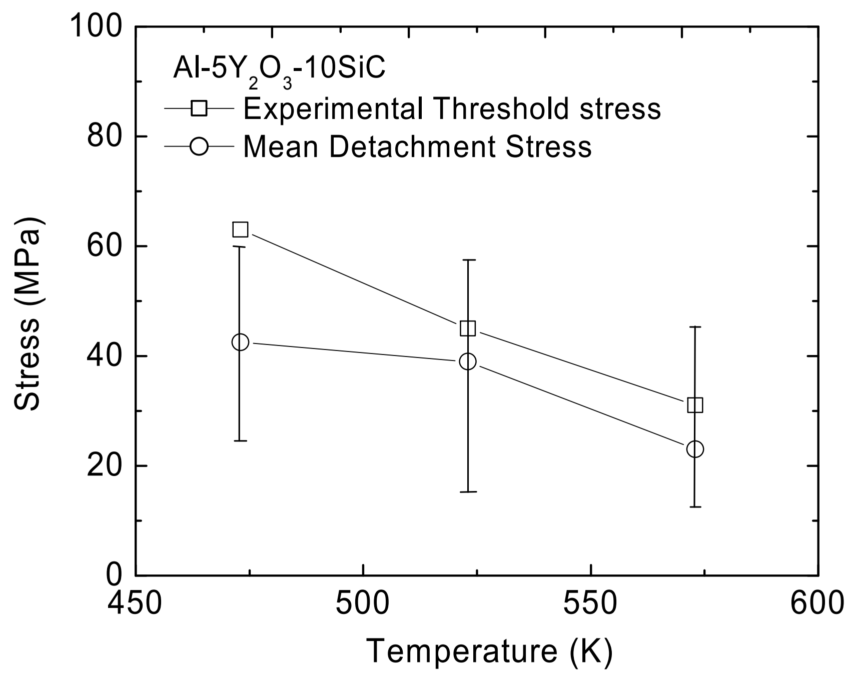
(a-f) Images captured from a video sequence recorded during the in situ straining. Dislocation movement through the array of Y_2O_3 particles at 250 °C (Deshmukh, Mishra and Robertson, 2010)

Background – In-situ TEM

Detachment Angle Measurement and Threshold Stress





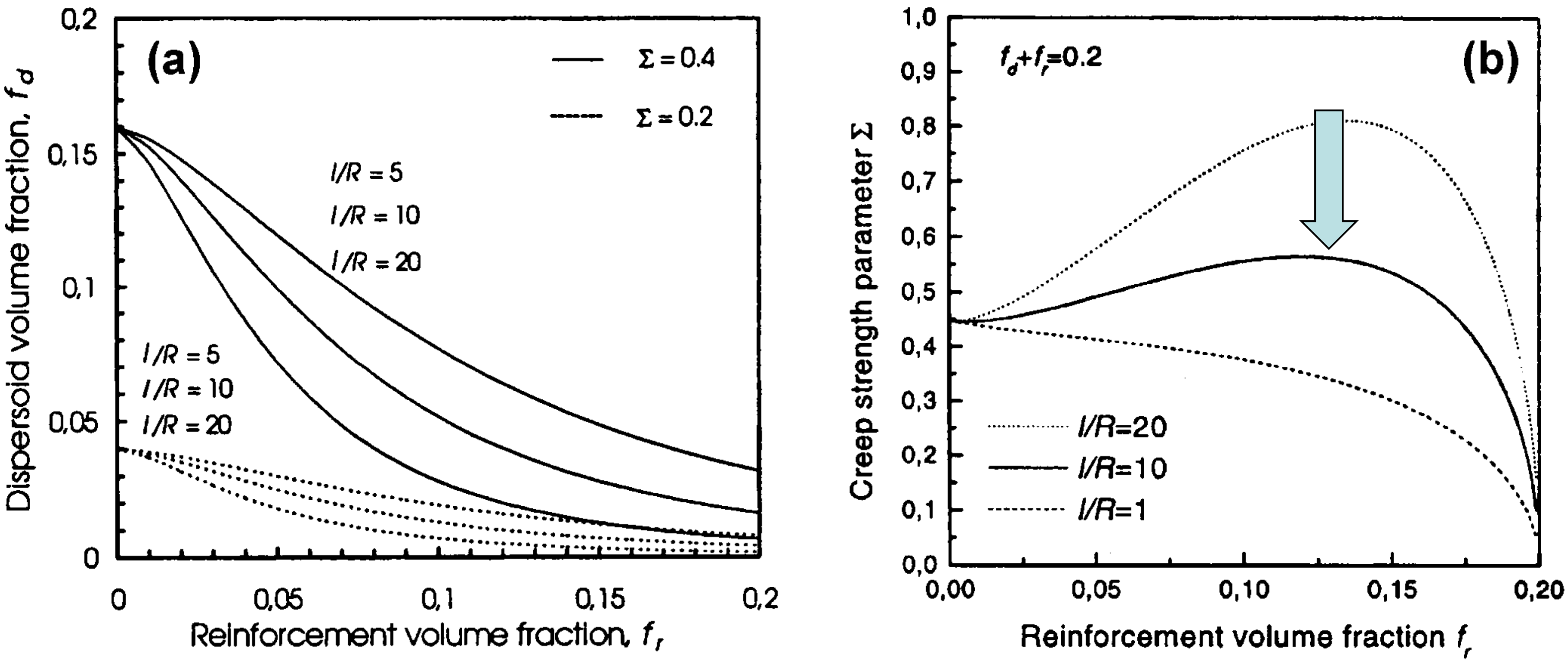


Motivation and Path Forward

Synergy among strengthening mechanisms: Can 2+2 be greater than 4?

- Rosler and Baker (2000) have proposed a theoretical concept for the design of high temperature materials by dual-scale particle strengthening
- The creep strength parameter, ∑, is defined as

$$\Sigma = \sqrt{f_d}\left(1+2(2+l/R)f_r^{3/2}\right)$$

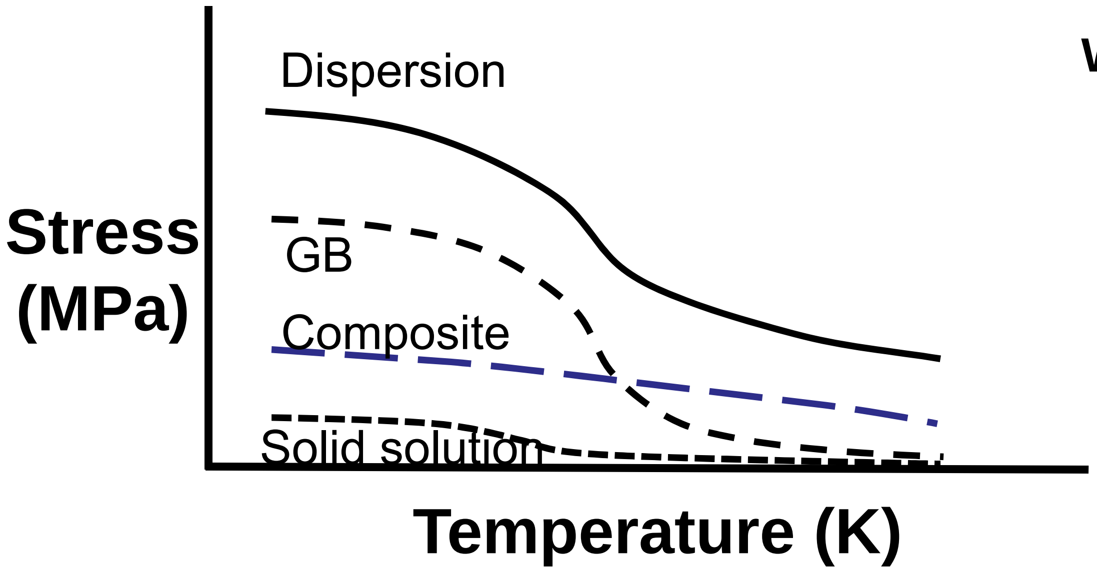


Discussion of Strengthening Mechanisms

There are four major components to strengthening in the nanostructured nickel based alloys produced by mechanical alloying:

- grain boundary strengthening,
- solid solution strengthening
- dispersion strengthening, and
- composite strengthening.

Effect of temperature



What are the additivity rules?

$$\sigma_{alloy} = \Sigma \sigma_i$$

$$\sigma_{alloy} = \sqrt{\Sigma(\sigma_i)^2}$$

$$(\sigma_{alloy})^k = \Sigma \sigma_i^{\,k}$$

Proposed Microstructure

Develop dual-scale strengthened Ni-Cr-Al_2O_3 alloys
The chosen alloy system has:

- Cr for solid solution strengthening
- nano Cr_2O_3 and/or CrN particles of 2-3 nm diameter for dispersion (currently using nano-Y_2O_3) strengthening
- submicron Al_2O_3 of 0.5-1 micron diameter for composite strengthening through increase in modulus

What is the level of synergy?

- Does the load transfer effectively enhance the creep life for equiaxed reinforcement?

Overview of Proposed Work

OBJ1: Microstructural Optimization

1A. Definition of design goals (UNT-UI-NETL) and material parameter constraints (UNT)
Strength, ductility, creep, residual stresses

1B. Identification of theoretical and phenomenological models (UNT)
Theoretical equations, data sets, empirical relationships

1C. Development of Genetic Algorithm optimization scheme (UNT)
Fitness function, Pareto-optimal solution sets, computational parameters

1D. Computer Simulation of Dislocation Motion for Visualization (UNT)
Multiple obstacles, particle size, particle shape, particle distribution

OBJ2: Develop Ni-Cr-Al_2O_3 with Dual-Scale Microstructure

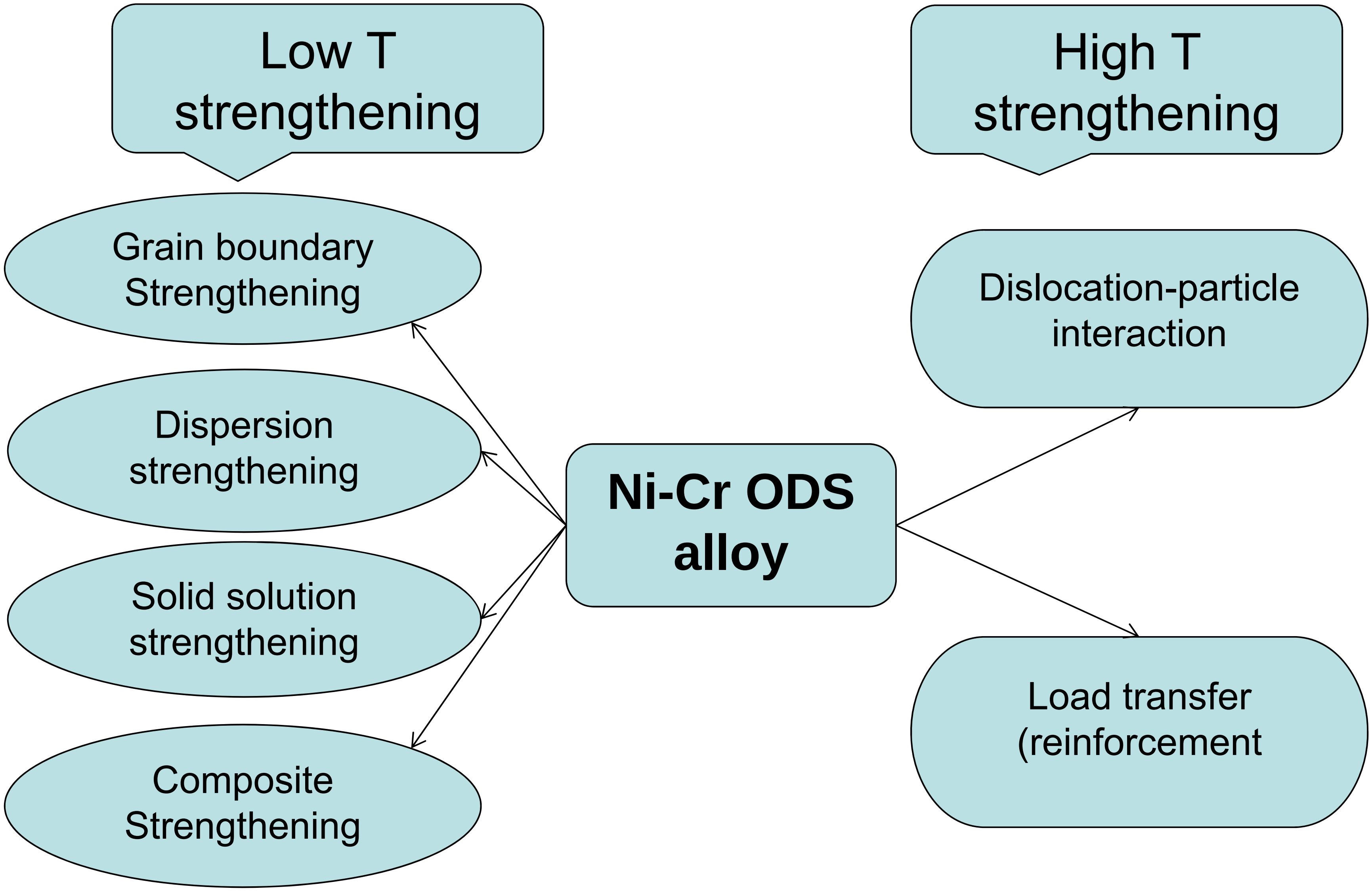
2A. Processing of GA optimized material (UI)
Milling, degassing and compaction, forging

2B. Experimental validation: Microstructure and Mechanical Properties (UNT and UI)
SEM, TEM, X-ray, hardness, tensile, creep

OUTCOME: Integrated Approach for 'Materials by Design'

Computational part

Strengthening Mechanisms



Low temperature strength

Strengthening mechanism	Equation
Grain size strengthening	$\sigma_y = \sigma_0 + Kd^{-0.5}$
Solid solution strengthening	$\Delta\sigma_s = \left(\sum k_i^{\frac{1}{n}} c_i\right)^n$
Dispersion strengthening	$\Delta\sigma_p = \frac{Gb\sqrt{f_d}}{d_p}$
Composite strengthening	$\sigma_c = V_p\sigma_p + V_m\sigma_m$
Load transfer coefficient	$\Lambda \approx 1 + 2\left(2 + \frac{l}{R}\right) f_r^{\frac{3}{2}}$

High Temperature strength

Dislocation creep

Modified power law creep [1]

$$\dot{\varepsilon} = 8.3 * 10^8 \frac{DGb}{k_B T}\left[exp\left(-104\sqrt{\frac{b}{\lambda}}\right)\right]\left(\frac{\sigma' - \sigma_0}{E}\right)^5$$

$$\sigma' = \sigma/\wedge$$

Threshold stress

Dissociation and positive climb model [2]

$$\sigma_0 = 0.002\, G\left(\frac{b}{r}\right) exp\left(20\frac{r}{\lambda}\right)$$

1. R. S. Mishra and A. K. Mukherjee, Light weight alloys for aerospace application III, TMS, (1995), 319
2. R.S. Mishra *et al*., Philosophical Magazine A,1994, 69 (6), 1097-1109

GA optimization work

Cost function

$$J = \frac{\left[\sum_{i=S,D,HTS} w_i \left|\left(\frac{P_i}{(P_i)_{desired}}\right) - 1\right|\right]}{n}$$

Various considerations were taken in order to minimize the cost function:

- 100 Individuals were considered in each generation.
- Rank scales were used for the fitness scaling. The rank of the fittest individual was 1, the next fittest was 2 and so on.
- Roulette method was used as a selection function to choose parents for the next generation.
- 10 best individuals survived to the next generation.
- Probability of crossover was chosen 0.85 and rest were produce via mutation.
- The optimization was running until 100 generations were completed or the cost function did not vary significant for 25 successive generations.

Notation used for variables:

- [w_S w_D w_{HTS}]= Weight factors for low temperature strength, ductility and high temperature strength properties.
- r (nm) is the radius of dispersoids particles.
- r_f (nm) is the radius of reinforced particles.
- f_r (%) is volume fraction of reinforcement.
- f_d (%) is volume fraction of dispersoids.

The optimization was carried out for two conditions:

I: 15 nm ≤ r ≤ 20 nm , 300 nm ≤ r_f ≤ 400 nm , f_r ≤ 15 %
II: 2 nm ≤ r ≤ 4 nm , 500 nm ≤ r_f ≤ 1000 nm , f_r ≤ 15 %

Desired properties

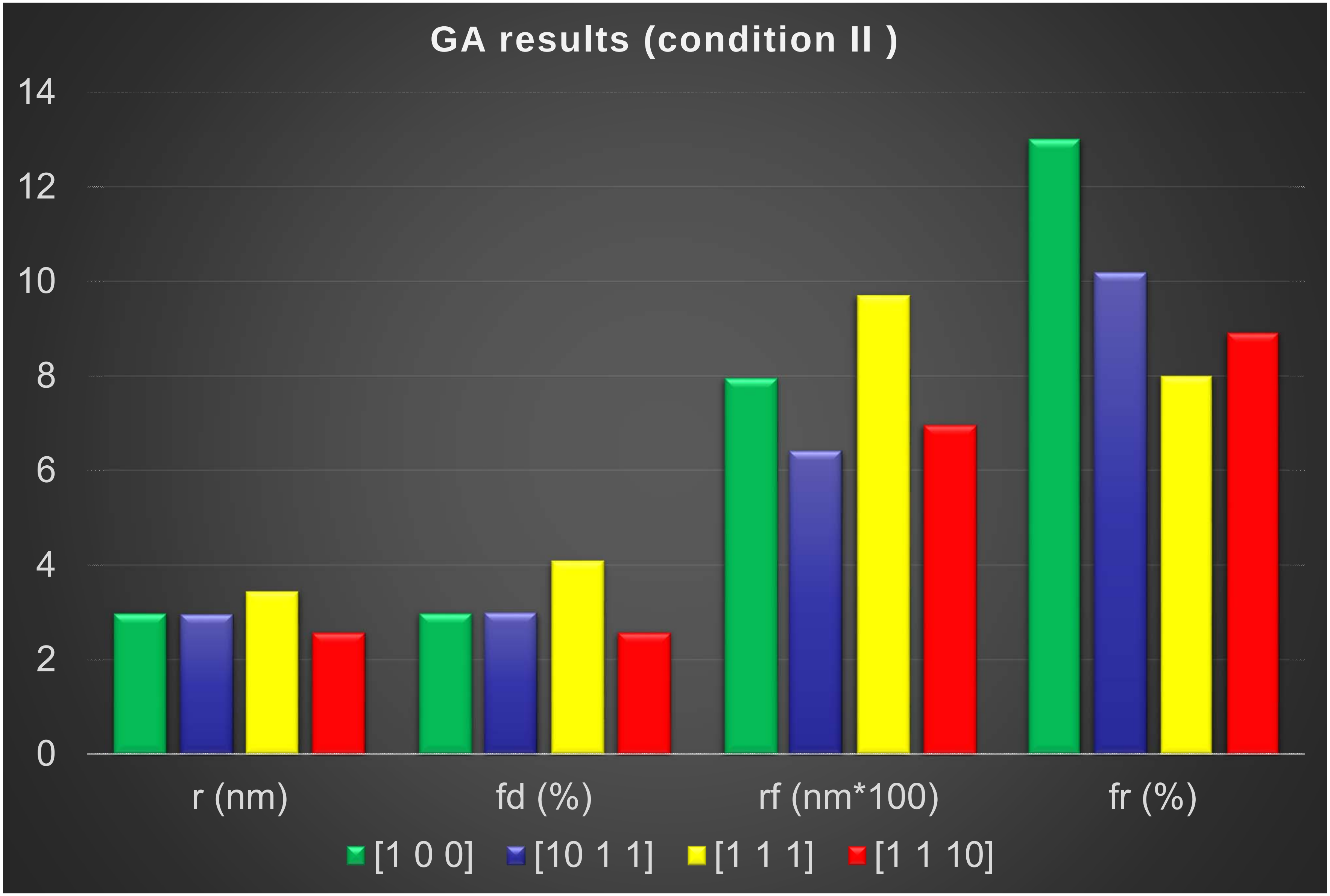
- low temperature - 900 MPa
- ductility - 10 %
- high temperature strength - 100 MPa

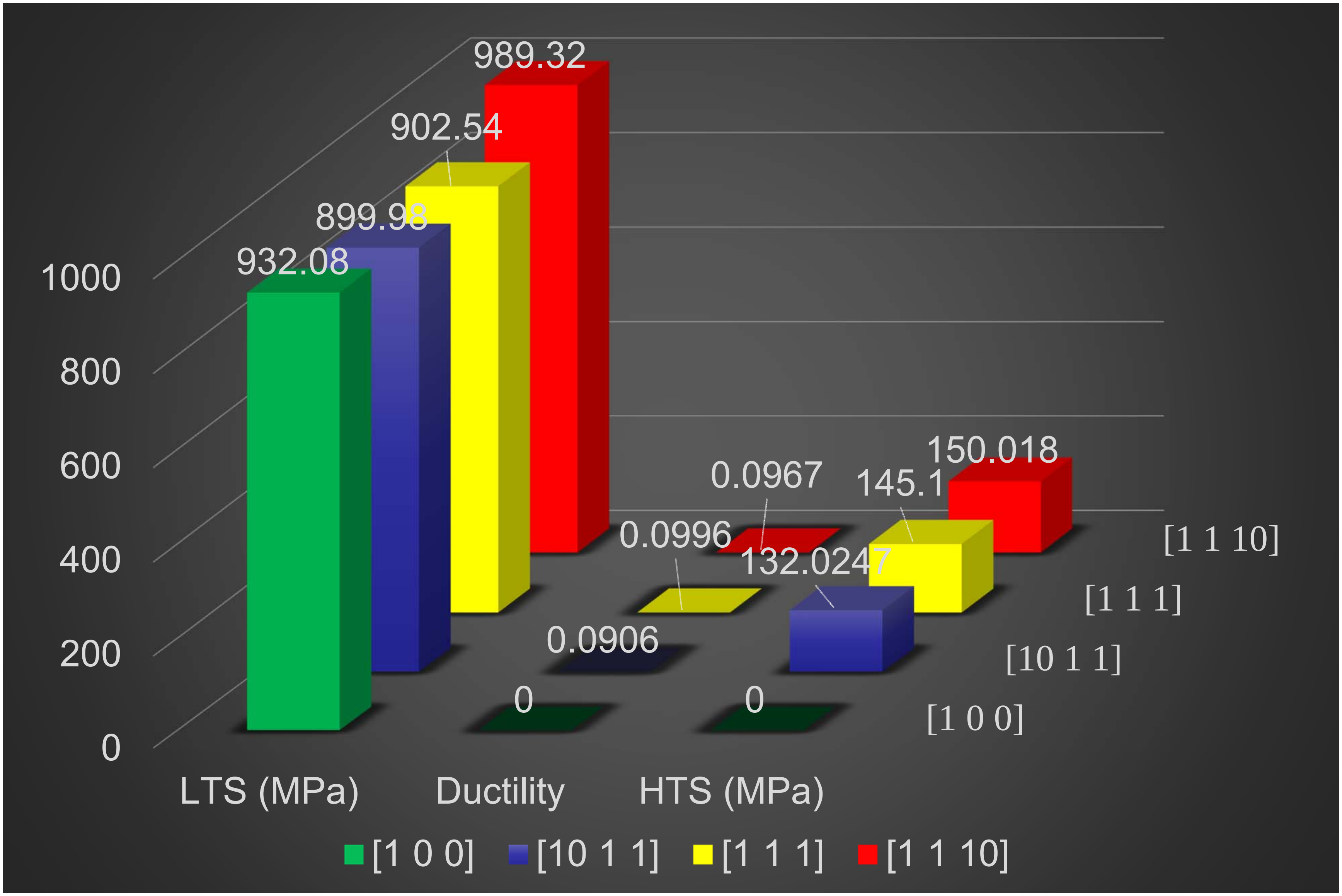
G=76 GPa, σ_o=17.4 GPa, K= 0.236 $MNm^{-3/2}$, b= 0.249 nm, T=1073 K, $\dot{\varepsilon} = 10^{-9}\ s^{-1}$

GA results

II: 2 nm ≤ r ≤ 4 nm , 500 nm ≤ r_f ≤ 1000 nm , f_r ≤ 15 %

Case	[1 0 0]	[10 1 1]	[1 1 1]	[1 1 10]
r (nm)	2.997	2.961	3.44	2.578
f_d (%)	3	3	4.089	2.578
r_f (nm)	797	642	971	697
f_r (%)	13.011	10.199	8	8.917
LTS (MPa)	932.08	899.98	902.54	989.32
Ductility	-	0.0906	0.0996	0.0967
HTS (MPa)	-	132.0247	145.10	150.018


GA results (condition II)
14
12
10
8
6
4
2
0
r (nm)
fd (%)
rf (nm*100)
fr (%)
[1 0 0]
[10 1 1]
[1 1 1]
[1 1 10]


989.32
902.54
899.98
932.08
1000
800
600
400
200
0
0.0967
150.018
145.1
0.0996
132.0247
0.0906
0
0
[1 1 10]
[1 1 1]
[10 1 1]
[1 0 0]
LTS (MPa)
Ductility
HTS (MPa)
[1 0 0] [10 1 1] [1 1 1] [1 1 10]

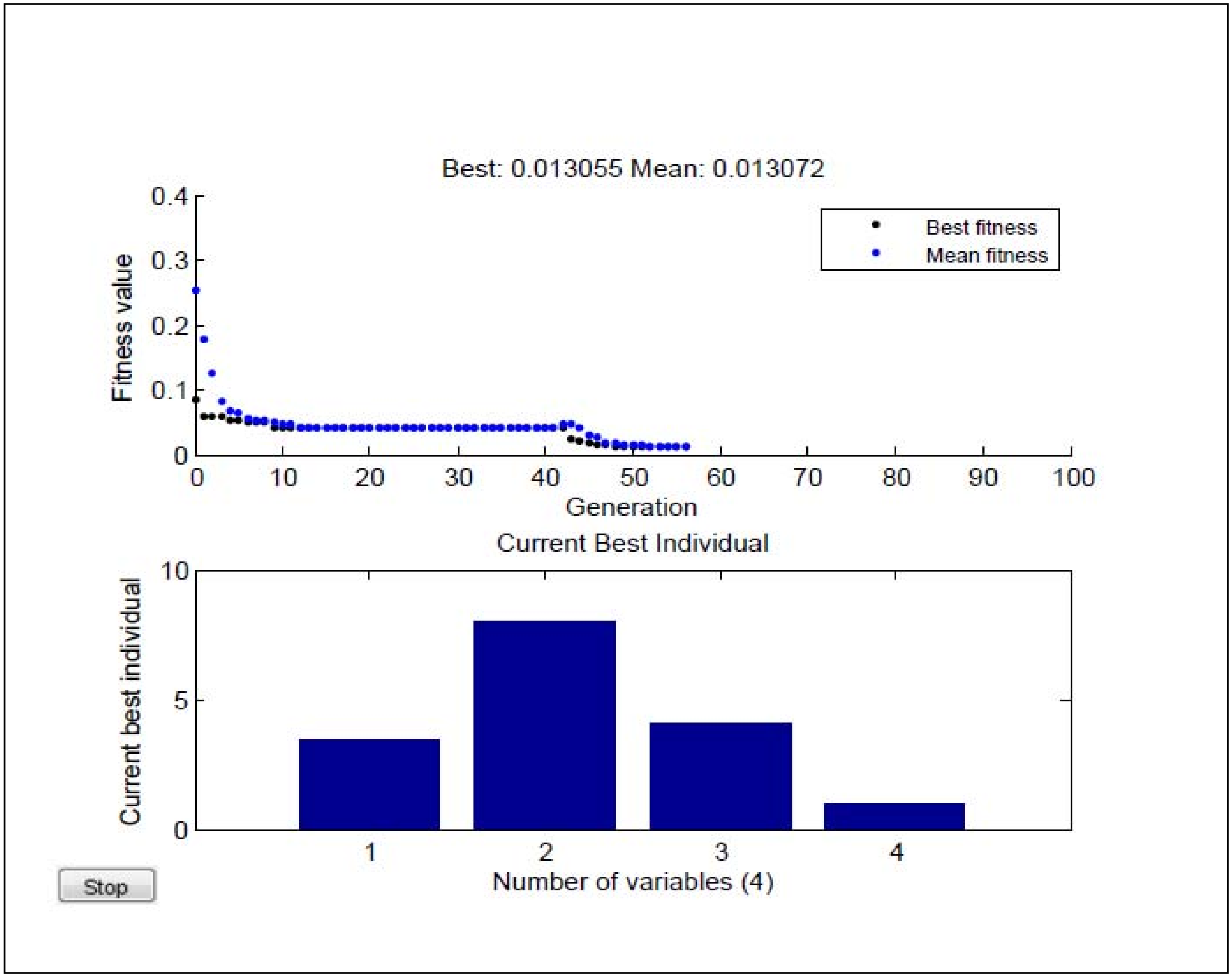


Fig. 2 GA plots for case [10 1 1]

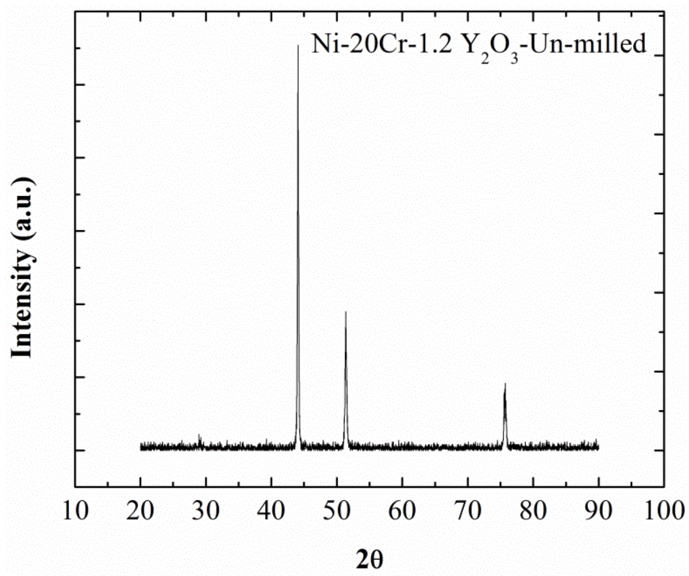
Summary for computational part

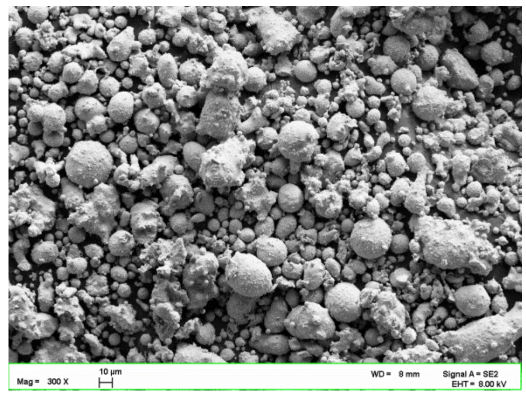
- Compilation of relevant theoretical and phenomenological model was done for low temperature strength, ductility and high temperature strength.
- The appropriate models were selected for further GA optimization work.
- The initial results showed:

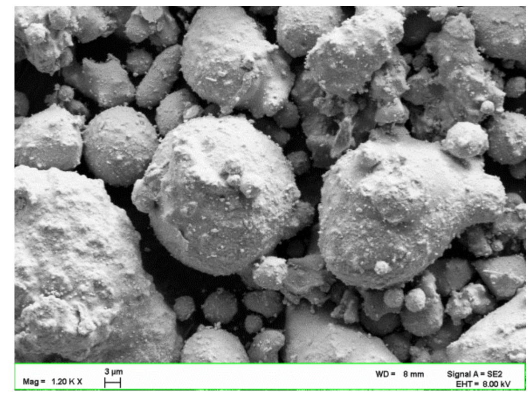
Condition I	Dispersoid radius (nm) ~ 15
	LTS (MPa) ~ 700
	HTS (MPa) ~ 40
Condition II	Dispersoid radius (nm) ~ 3
	LTS (MPa) ~ 900
	HTS (MPa) ~ 145

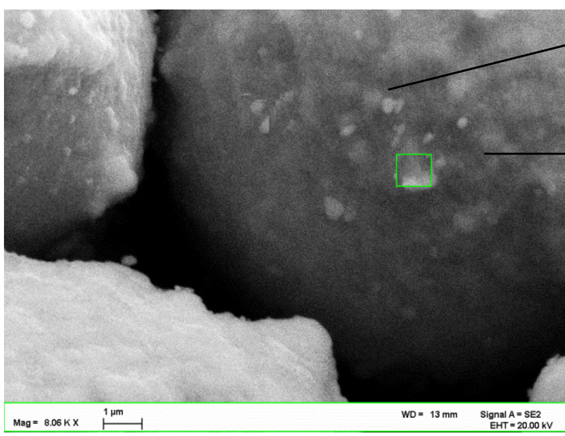
Experimental Part

Ni-20Cr-1.2Y_2O_3 - characterization









Y_2O_3

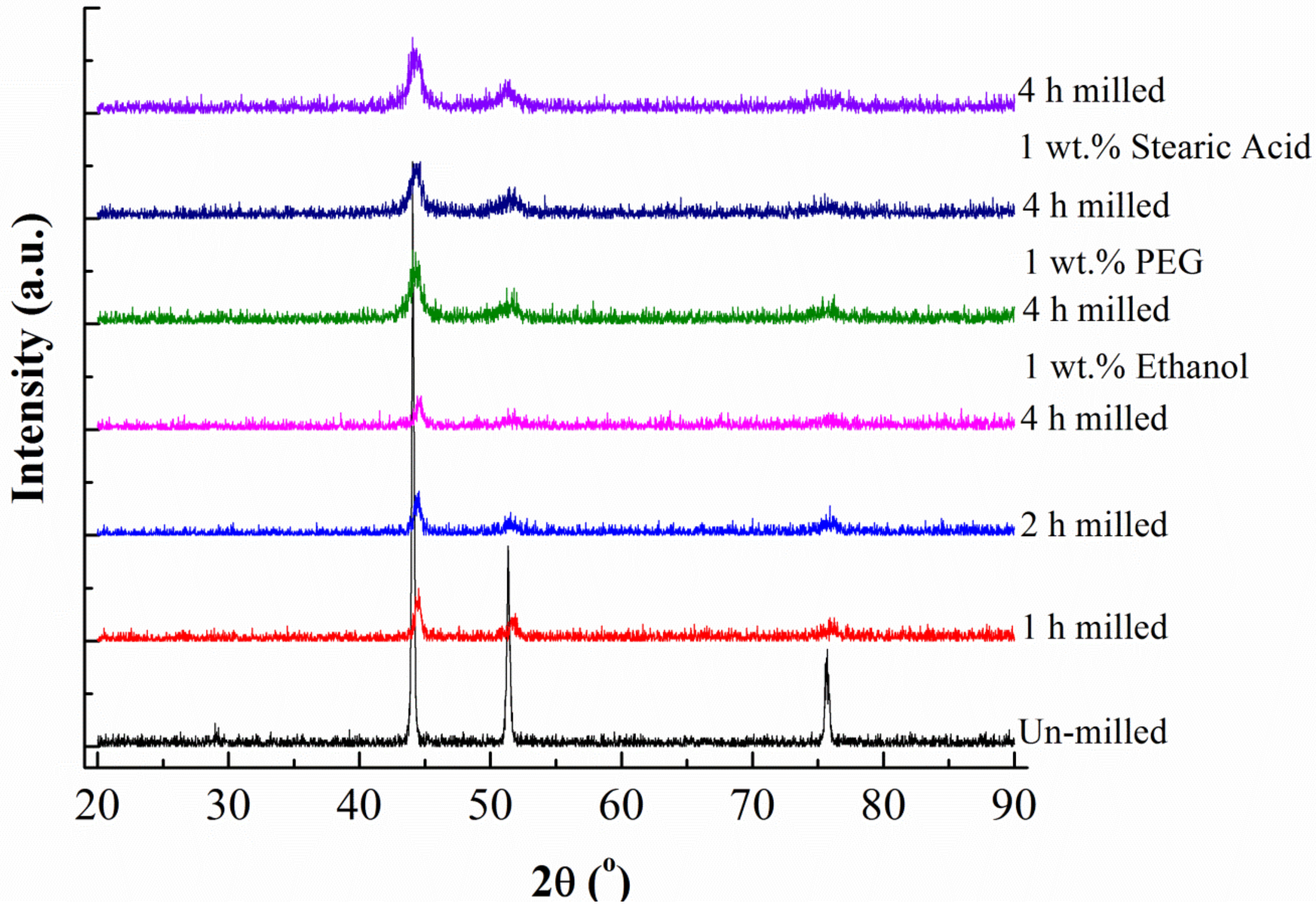
Element Line	Net Counts	Net Error	Element Wt.%	Wt.% Error	Atom %	Atom % Error
Si K	2675	+/-85	2.469	+/-0.079	5.061	+/-0.161
Cr K	16634	+/-222	19.383	+/-0.258	21.465	+/-0.286
Fe K	592	+/-73	0.874	+/-0.108	0.901	+/-0.111
Ni K	30669	+/-306	67.620	+/-0.675	66.320	+/-0.662
Y L	7522	+/-152	9.655	+/-0.195	6.253	+/-0.126
			----------		----------	
Total			100.000		100.000	

- The mean powder particle size was 25 mm.
- The Ni powder particles were covered with yttrium oxide nanoparticles as indicated by EDS.

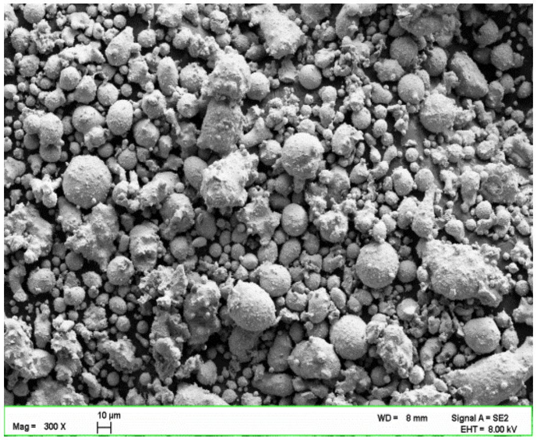
Milling experiments

- Milling was done for 1 h, 2 h and 4 h and the XRD were used to characterize them.
- XRD patterns showed that 4 h was not long enough to make the yttria peaks disappear.
- Significant peak broadening and peak shift to higher angles were observed after 1 h milling.

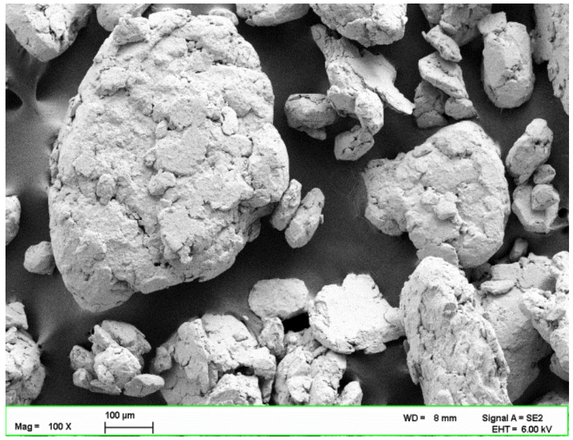
XRD patterns for milled Ni-20Cr-1.2Y_2O_3



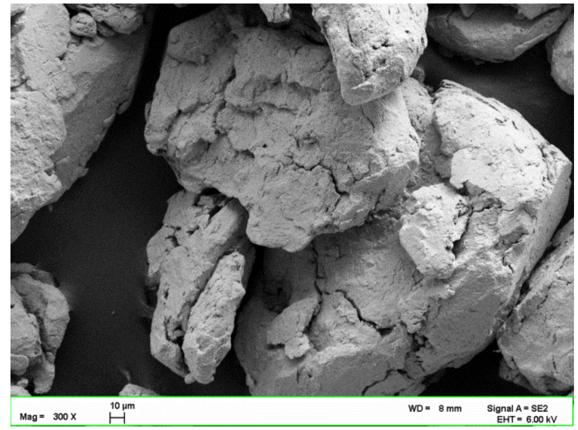
Particles agglomeration



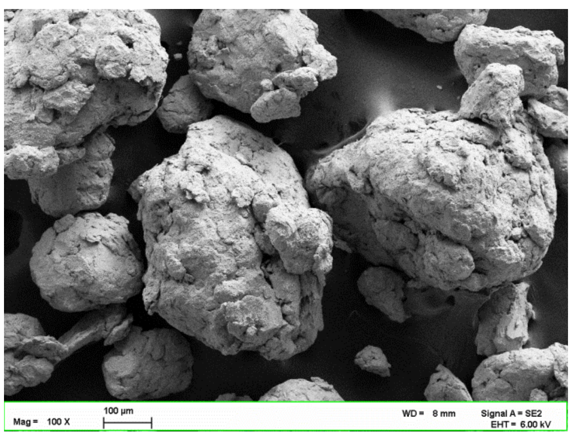
Un-milled



1 h



2 h

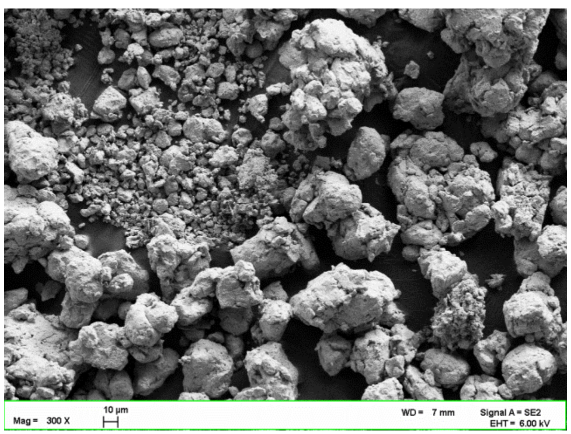


4 h

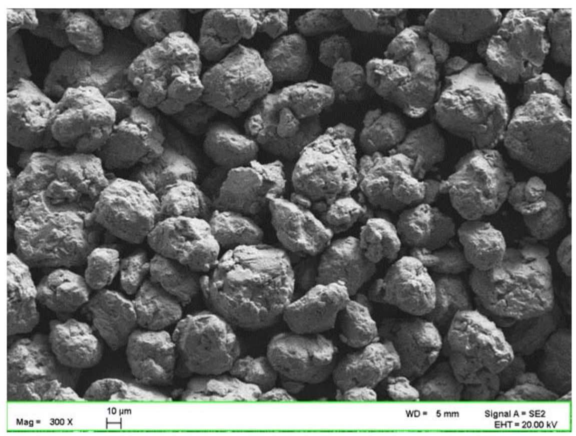
- Only after 1 h the mean particle size increased to 280 mm.
- Significant agglomeration happened in the milled powder
- Agglomeration will decrease the efficiency of mechanical alloying
- The fine particles increase the sintering efficiency and final density.
- Using a particle control agent (PCA) may decrease this agglomeration

Using PCA

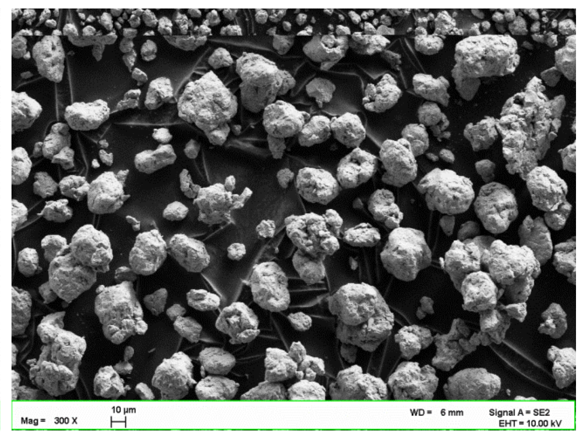
- In literature, ethanol, poly ethylene glycol (PEG) and stearic acid were used as PCA.
- 1 wt% of ethanol, poly ethylene glycol (PEG) and stearic acid were added to the powder mixture and milled for 4 h.
- The mean particle size of the milled powder deceased using PCA and the agglomeration decreased.
- The efficiency of stearic acid to minimize the agglomeration was more than ethanol and PEG.



4 h- Ethanol



4 h- PEG



4 h- Stearic acid

Summary for Experimental Work

- Ball milling experiments using a shaker mixer/mill (SPEX) of the Ni-20Cr-1.2Y_2O_3 (wt.%) alloy composition were carried out.
- Scanning electron microscopy (SEM) in conjunction with energy dispersive spectroscopy (EDS) was performed to characterize the morphology and chemical characteristics of the milled powder.
- It has been determined that steel balls of 5 mm diameter, a ball to powder ratio (BPR) of 10:1 and a milling time of 2 h are as optimal milling conditions. A 1wt.% stearic acid was added to the powder mass during ball milling to prevent powder agglomeration.
- The structural parameters under the optimum conditions were found to be as following: average crystallite size (14 nm), lattice strain (0.003%), lattice parameter (0.3536 nm) and mean powder size (33.6 μm).

Future Work

- Continue the GA effort
- Start dislocation simulation work
- Theoretical modeling/refinement of positive climb model
- Consolidation of ball milled powder
- Mechanical property evaluation

Thank You