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Award No. DE-FEOO08719

Synergistic Computational and Microstructural Design of Next-Generation High-Temperature Austenitic Stainless Steels

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❖ Project Goal(s)

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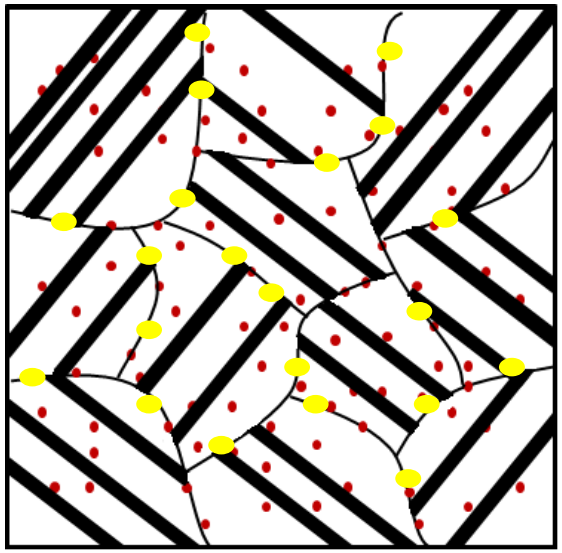
- Design new austenitic stainless steels (ASS) for advanced ultra supercritical combustion coal-fired power systems
  - ✓ High temperature strength
  - ✓ High ductility
  - ✓ Good creep resistance
  - ✓ Good high temperature oxidation/corrosion resistance

- Design of micro-alloying additions, heat treatment schedules, and microstructure
  - Cost-effective alternatives to Ni-base superalloys
  - Higher-temperature alternatives to ferritic steels

- Develop a robust ICME design/optimization framework for high temperature ASS.



Alloy + Microstructure Design

- Austenitic structure
- High density of low energy grain boundaries or nano-twin boundaries
- Nano-scale precipitates, intermetallics, laves phases stable at high temperature
- Formation of alumina surface oxide

❖ Strategy—Computer-Aided Alloy Design

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- Optimization of micro-alloying additions for desired microstructure and given performance criteria:
  - Single bulk phase, i.e. austenite
  - Control SFE and enhanced twinning ability
  - Alumina formation
  - Dissolvable carbides/carbonitrides (welding issue?)
  - MC instead of $M_{23}C_6$
  - High temperature intermetallics and laves phases
  - Very fine particles (control MC size with Nb, Ti, Zr, V, etc., nucleation at dislocations and twin boundaries)

- **Prediction of alumina-scale forming ability**

- **Prediction of twinning ability**

- Transformation kinetics of precipitate phases

In This Talk:

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- **Experimental determination of stability of deformation twinning nano-structures**
- Stacking Fault Energy Models and Data Analysis
- Thermodynamic/Kinetic Criteria for Alumina Formation
- GA-based Alloy Design

❖ Strategy--Microstructure Design

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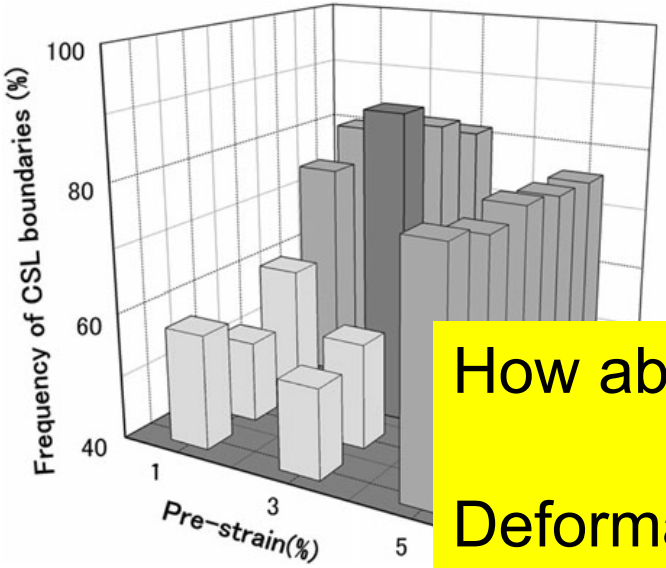
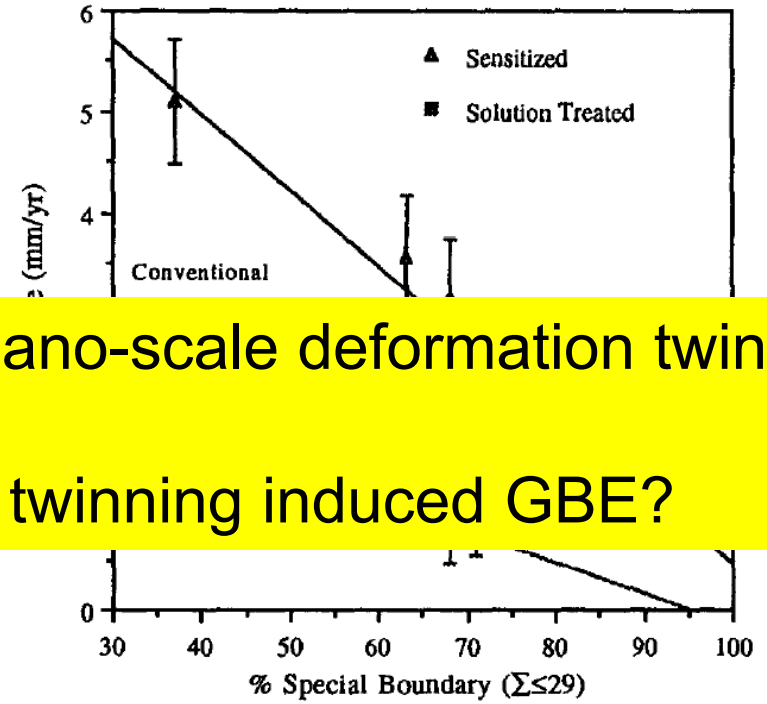
- Twinning induced Grain Boundary Engineering (GBE)



Effects of pre-strain and annealing temperature on the frequency of CSL boundaries in thermomechanically processed 321 austenitic stainless steel, cited from Kurihara et al.



How about nano-scale deformation twins?

Deformation twinning induced GBE?

References

Lin, P., G. Palumbo, U. Erb, and K. Aust, Scripta Materialia, 1995. 33(9): p. 1387-1392.

Kurihara, K., H. Kokawa, S. Sato, Y. Sato, H. Fujii, and M. Kawai, Journal of Materials Science, 2011: p. 1-6.

❖ Strategy--Microstructure Design

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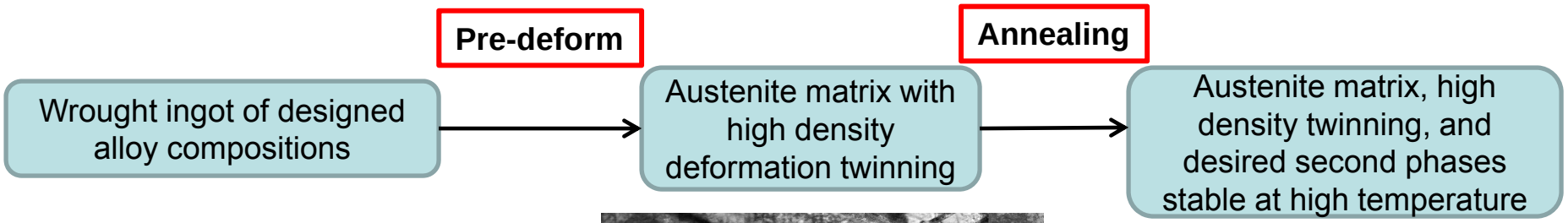
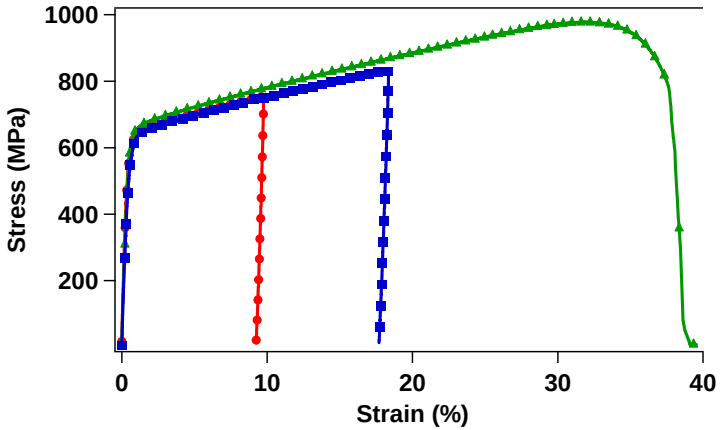
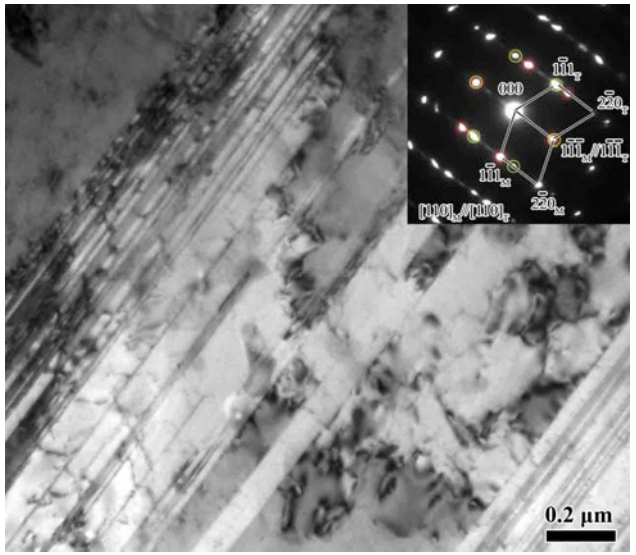
- Simple thermo-mechanical processing





316 Stainless Steel deformed



316 Stainless Steel
Heat-treated

❖ Questions and Challenges

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- Fundamental study of recovery and recrystallization (ReX) of deformation twins in low SFE steels in the presence of various densities of dislocations.
  - In polycrystal of 316 SS
- Role of in-situ carbides and nitrides of Ta, V, W, Cr during recovery and ReX in the presence of deformation twins? What is the optimum thermo-mechanical processing path?
- Control of particle size and distribution with micro-alloying control
- Multi-objective alloy optimization using genetic algorithms
- The role of deformation twins, laves phases, nano carbides, and intermetallic particles on creep and stress rupture behavior of designed steels.

❖ Materials studied so far

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Hadfield Steel	✓ Highly twinned {001}/{111} texture
	× Evolution of second phase at high temperatures
316N SS	✓ Fully austenite
	× No twinning
316 SS	✓ Fully austenite
	✓ Twinning
	× No alumina scale formation

Study: deformation-twin thermal stability and their effect on recrystallization and grain boundary character distribution

Alloys selected based on literature

Alloy 1	✓ Fully austenite
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	× Uncontrollable Ti-Nb carbo-nitrides and AlN precipitation

all in wt%	Fe	Ni	Cr	Mn	Nb	Si	Al	Ti	Mo	V	C	N	B
Alloy 1	Ba.	20	14	2	0.86	0.15	2.5	0	2.5	0	0.08	0	0.01
Alloy 2	Ba.	12	14	10	1	0.2	2.5	0.3	2.5	0.5	0.08	0.01	0
Alloy 3	Ba.	17	14	10	1	0.2	2.5	0.3	2.5	0.5	0.08	0.01	0

❖ Twinning in Polycrystals

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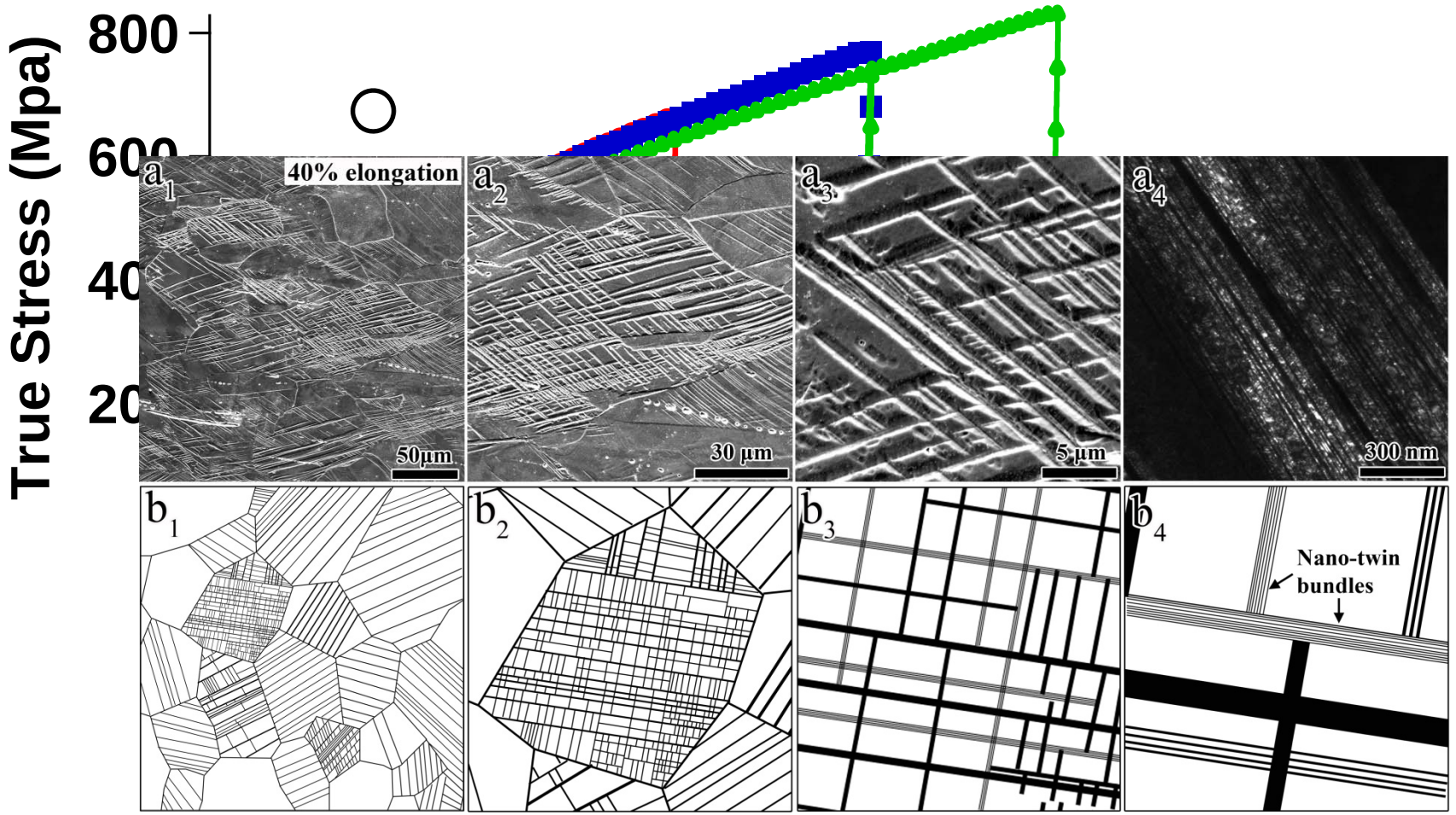
316 Stainless Steel, 40% Tension at RT



❖ Twinning in Polycrystals

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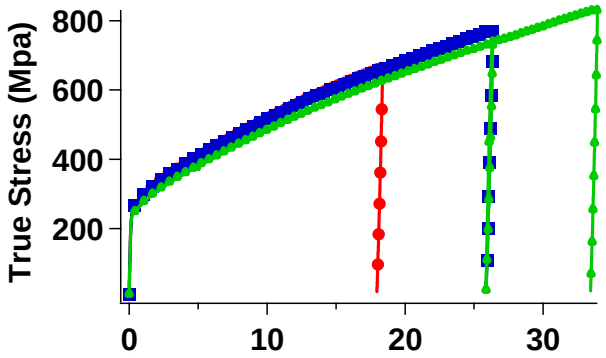
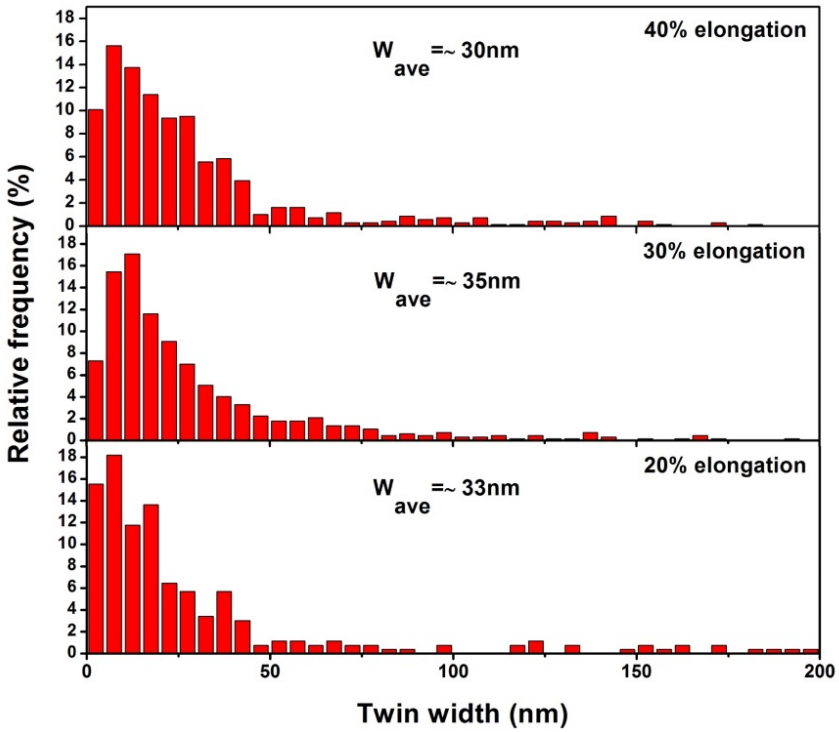
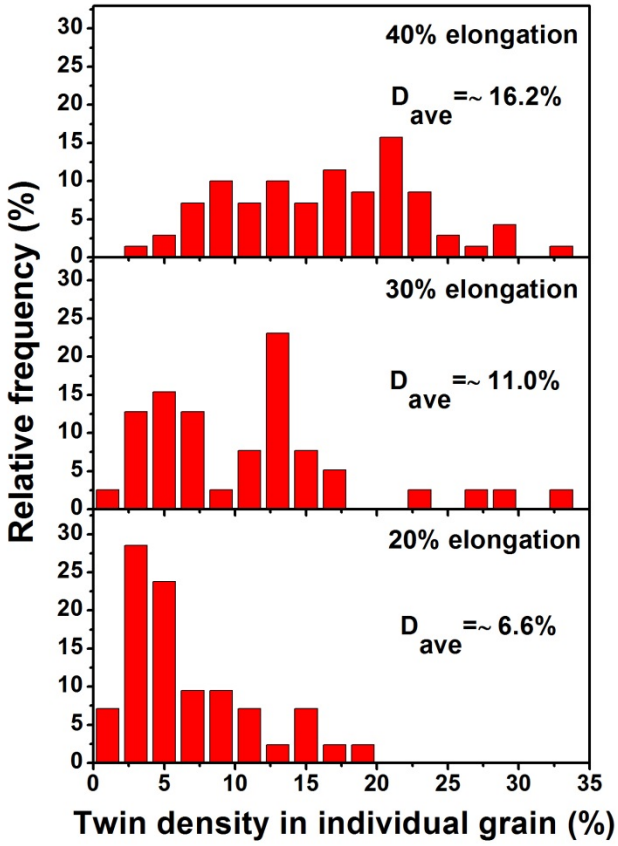
316 Stainless Steel, Tension at RT







	20%	30%	40%
Grains with twins (%)	62.6±4.6	77.3±3.1	79.5±4.3

❖ Twin Thermal Stability During In-situ TEM Heating

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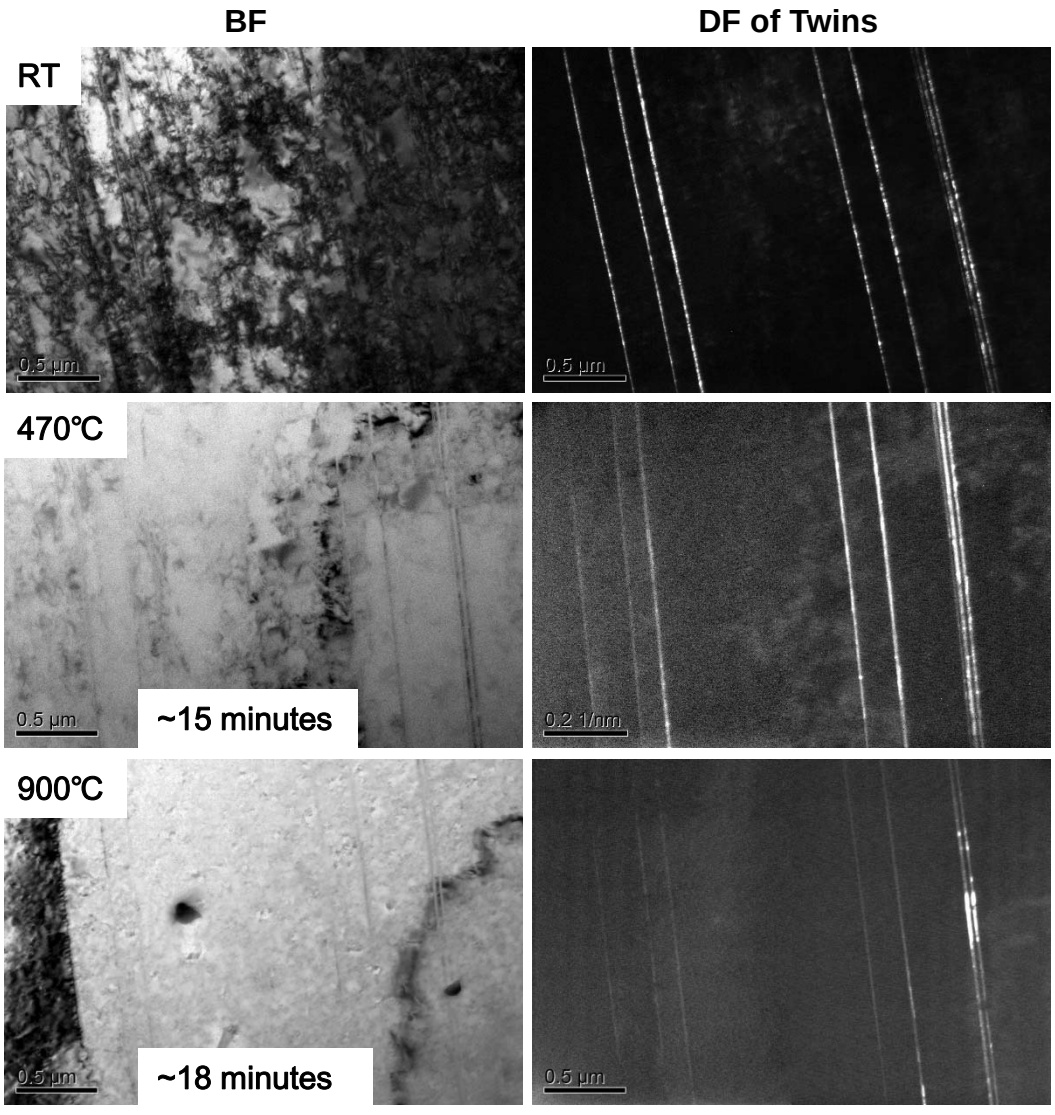
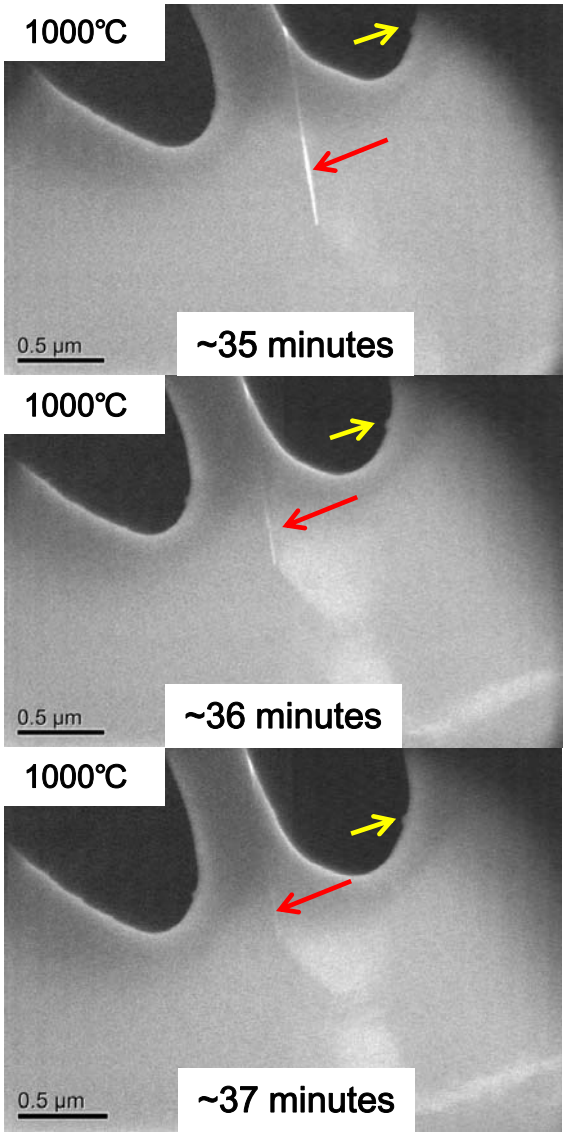
316 Stainless Steel, Strained 20%





❖ Twin Thermal Stability

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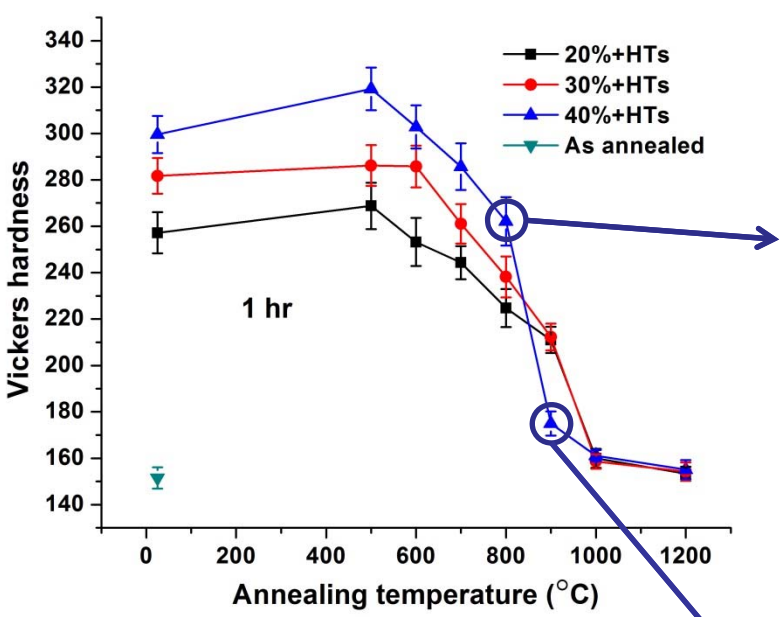
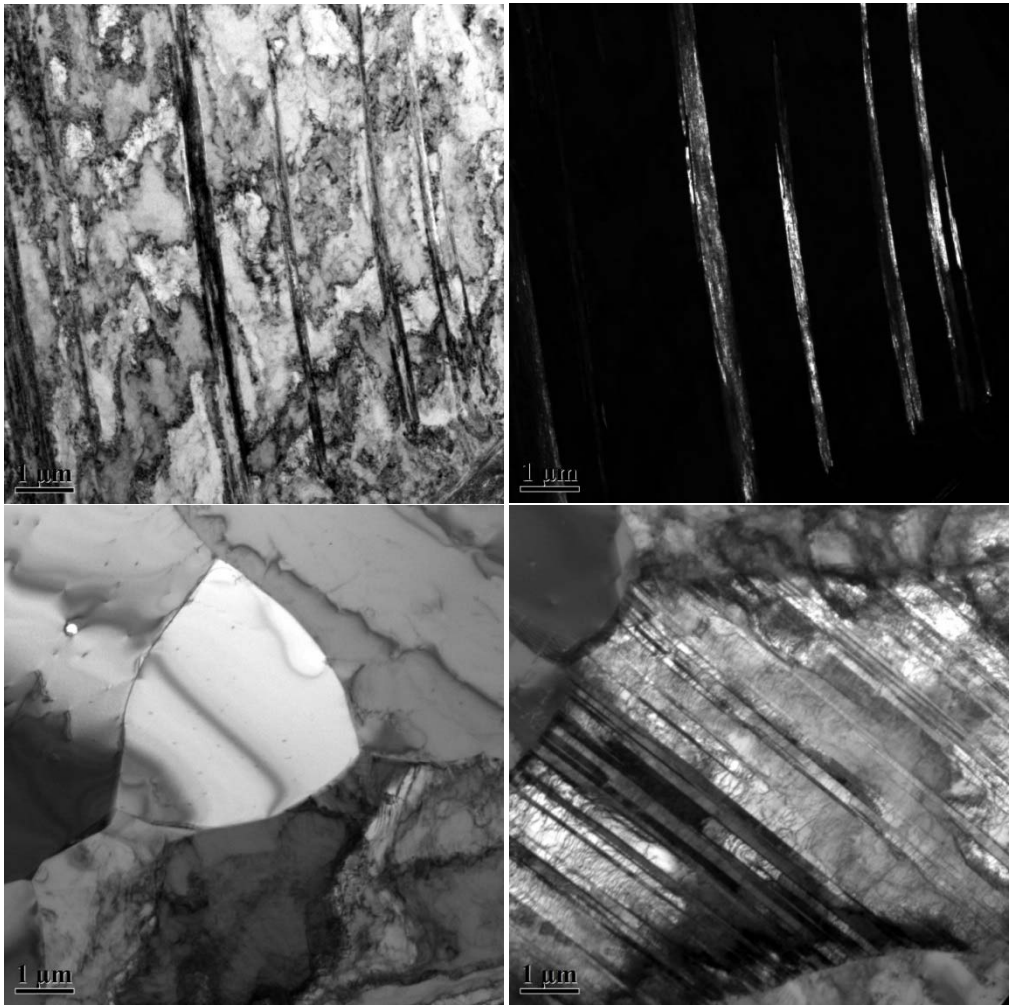
316 Stainless Steel, Tension at RT





❖ Twin Thermal Stability

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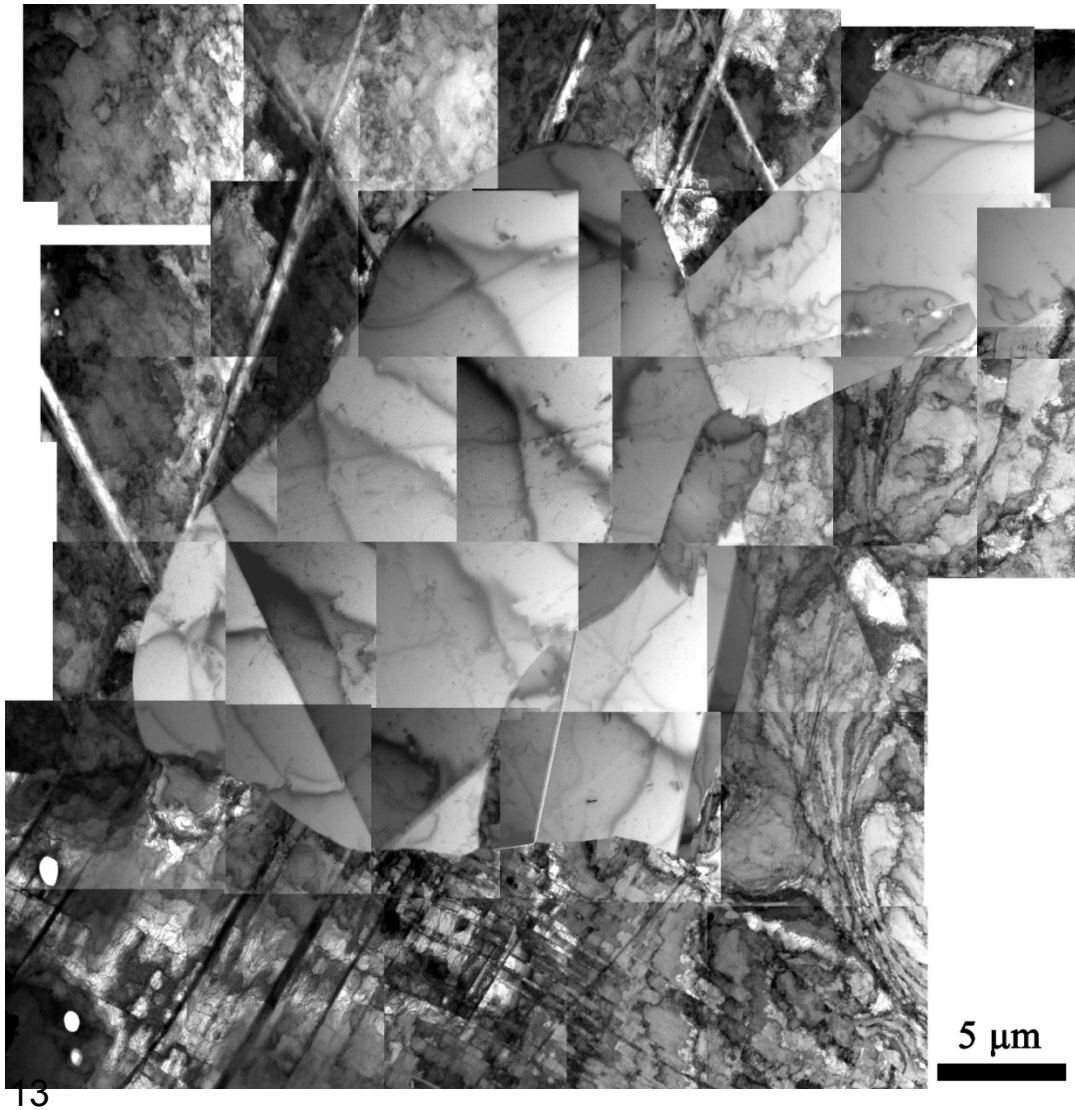

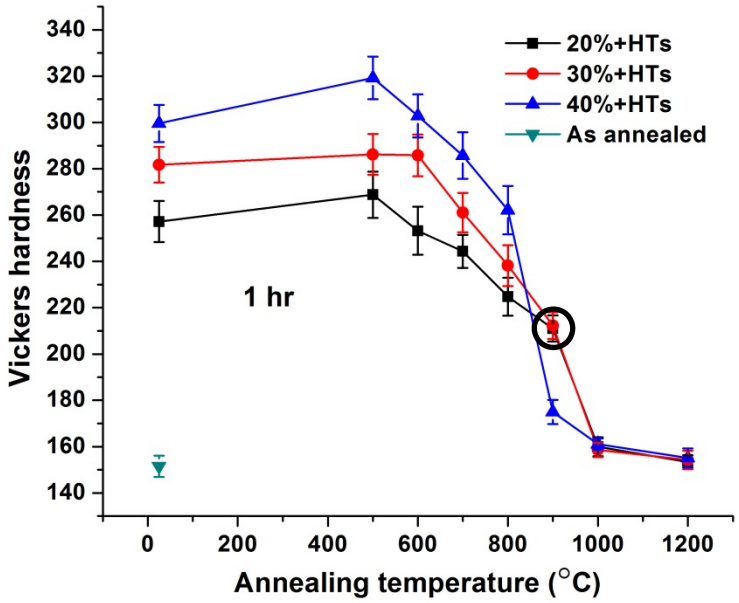

❖ Twin Thermal Stability

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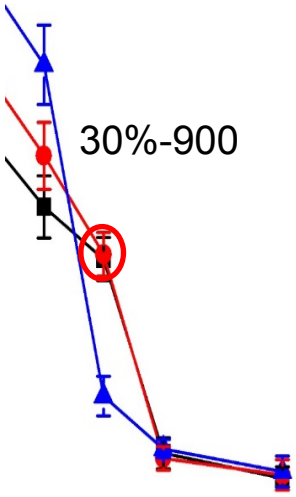

❖ Twinnability: Summary & Future Work

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1. The twin density increases with the increasing amount of strain.
2. The twin width is still at nano-scale despite different strain levels.
3. From in-situ and in-furnace heat treatments: deformation twins are stable up to 900˚C, under zero stress, for one hour.

o Observed thermal stability of these nano-twins constitutes a promising strategy for strengthening stainless steels at elevated temperatures.

❑ Create deformation twins, anneal away the dislocations, deform again to increase twin density.

❑ Study mechanical behavior and creep response of twin-strengthened steel, under load and higher temperatures.

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all in wt%	Fe	Ni	Cr	Mn	Nb	Si	Al	Ti	Mo	V	C	N	B
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❖ Prediction of Stacking Fault Energy as a Function of Alloying Additions

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Models:

Experimental Measurements
- (A. Dumay 2006)
- (Schramm 1975)
- (Xing Tian 2008)
- Many more

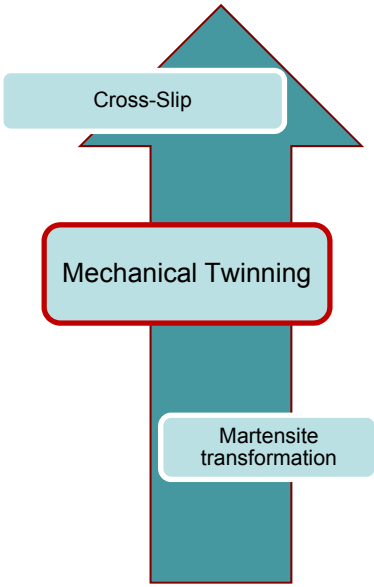
Theoretical Predictions
- (Cohen 1976)
- (Mullner 1998)
- (Jacques 2010)
- (Vitos 2011)
- (Q. Lu 2013)
- (K. Ishida 1976)
- Many more

Effects on SFE:

1. Alloying elements
2. Temperature
3. Interstitials

Prediction:

SFE → High
SFE → Low



❖ Relevant to creep, strain deformation, annealing twins, formation of dislocations, stress corrosion cracking, phase transformation stability, and electron/vacancy density, but we want to optimize SFE to ensure formation of deformation twins

❖ Challenges in Measuring/Predicting SFE

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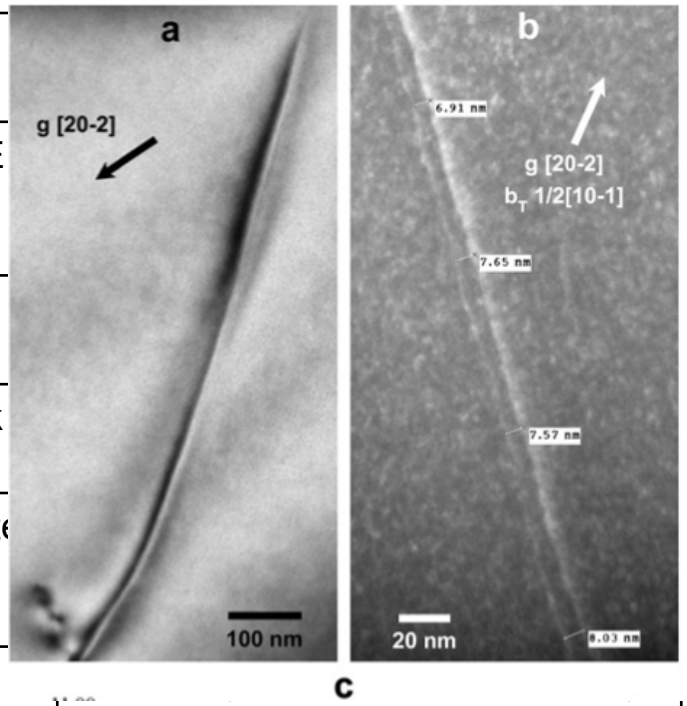
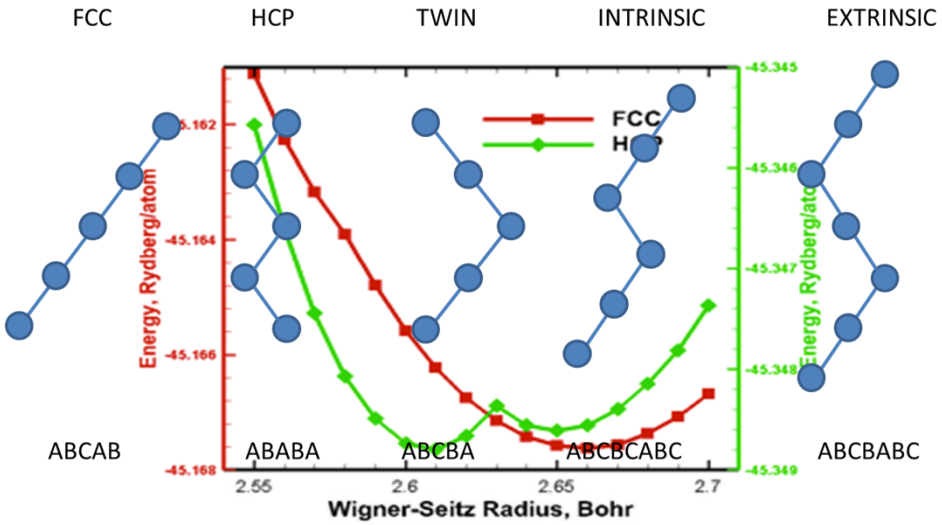
Method	Uses	
TEM	Traditional direct measure of SFE through node radii.	
Weak beam	Direct measure between dissociated partials	
XRD	SFE from peak position and peak broadening	
HREM	Uses both transmission and scatte interference for high atomic resolution	
Ab-initio	DFT calculations	interstitial effects. Verification from experiment needed
Thermodynamics	Many models:	Thermodynamic parameter guess work. System specific
EAM	For pure metals or binary	Limited applicability



Prediction of SFE-ANNI Model



Axial Next Nearest Neighbor Interaction (ANNI) Model:

$$E = E_0 - J_1 \sum_i S_i S_{i+1} - J_2 \sum_i S_i S_{i+2} - J_3 \sum_i S_i S_{i+3}$$

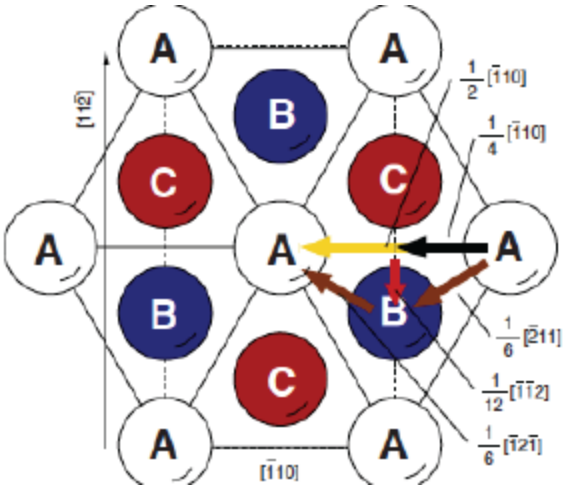
$$F_{SF} - F_0 = -4J_1 - O(J_2) \approx F_{HCP} - F_{FCC}$$

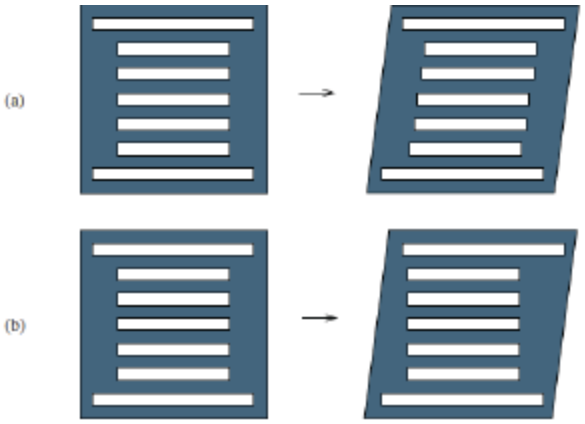
Method: EMTO-CPA

	μ^{FCC}	μ^{HCP}	γ_0	$\gamma_{M,RT}$	γ
$Fe_{74.5}Cr_{13.5}Ni_{12}$	1.61	0.00	7.03	30.71	37.75
[14]	1.62	0.00	8.50	36.20	44.60
$Fe_{70.5}Cr_{17.5}Ni_{12}$	1.54	0.00	6.67	29.84	36.51
[14]	1.54	0.00	-1.10	29.70	28.60
$Fe_{65.5}Cr_{17.5}Ni_{12}Mn_5$	1.32	0.00	7.19	26.97	34.15

Magnetic Entropic Contributions are Essential

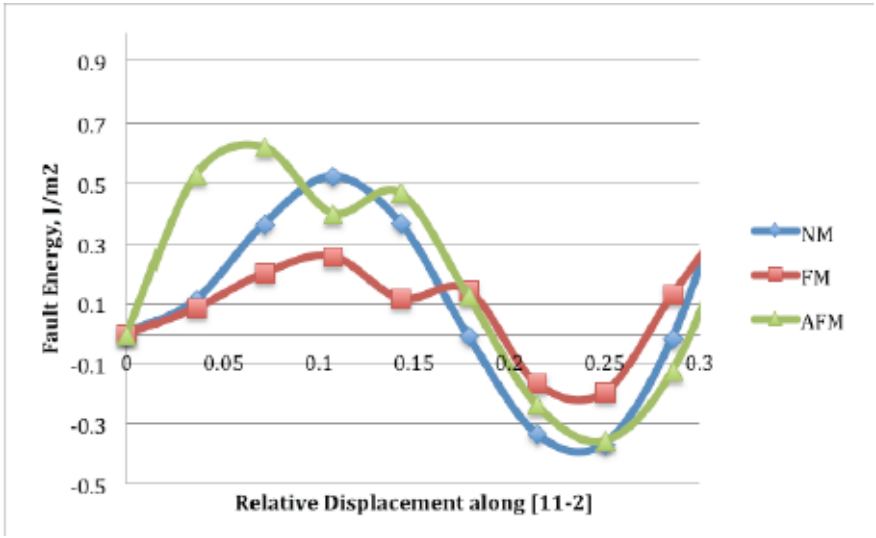
Prediction of SFE – *Ab Initio* Lattice Deformations





[Jahnatek et al PRB 2009]

Pure Fe



❖ Stacking Fault Energy -Challenges

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Incorporation of SFE into alloy design is essential

- Many attempts from literature to formulate temperature and alloying effect on SFE, from experiment and from theory, have had limited success
  - "Until today, no generally accepted method for the SFE calculation exists that can be applied to a wide range of chemical compositions" (Saeed-Akbari, 2013)
  - high error of uncertainty- values reported in the 1960's and early 1970s are, in general 20-30% overestimated (Campos, 2008)
  - "In summary, there is no agreement on accuracy of SFE values obtained, and perhaps no better than about 20 pct" (Siems et al)
  - Theoretical big discrepancy with carbon effect (either no effect or huge effect)- relaxation time for carbon diffusion, and how carbon interacts with the SF
  - "The dependence of the SFE on…carbon…is not yet fully understood, and different tendencies have been found by different authors" (Mujica 2012)

❖ Data Mining Approach (SFE)

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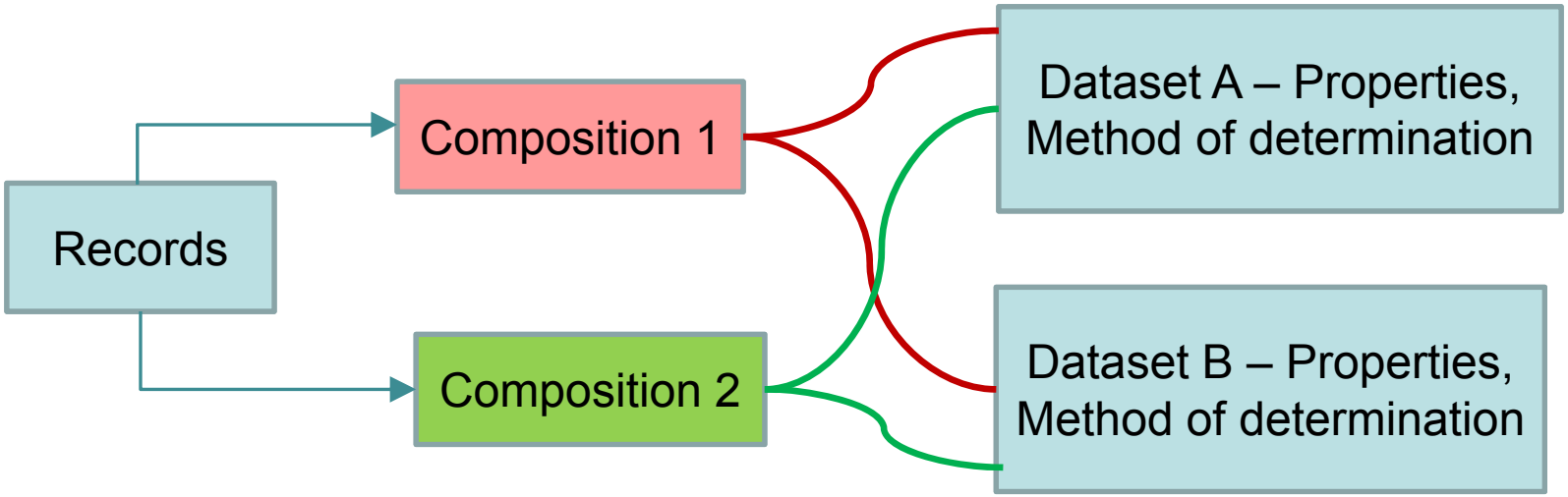
Database Builder



Modular software design

- Adaptable
- Efficient
- High throughput

Data capture

- User input
- Automated
- Theoretical
- Experiment

Analysis

- Neural Network
- Ab-initio

❖ Data Mining Approach (SFE)

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Experimental

SFE	Ni 10-16%	Cr 13-18%	Mn 0-4%	Nb 0-0.5%	Si 0-2%	Al * 0.2-6%	Mo 0-3%	C 0-0.08%
Increase	2.8	0.39 0.49	0.75	?		2	2.2	
Decrease		?		?	-2.0			-0.47 -2.1 -5.7

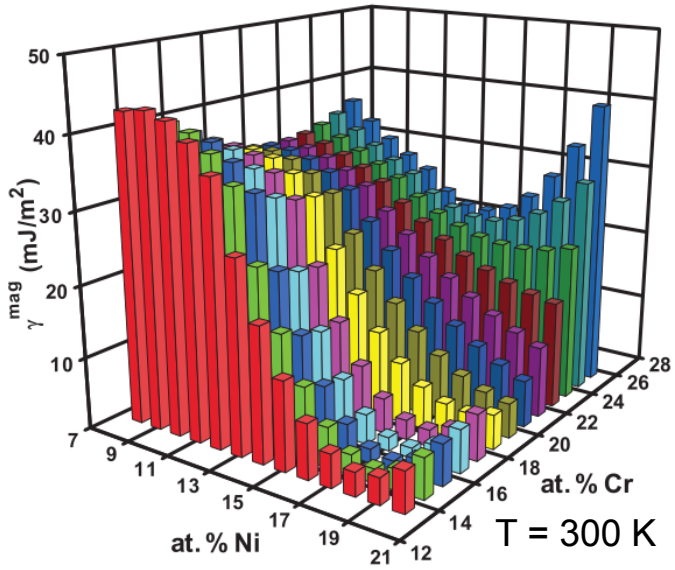
Examples - SFE trends based on preliminary literature Experimental/Theoretical data

Theoretical

SFE	Ni	Cr	Mn	Nb	Si	Al	Mo	C
Increase	✓			✓	?	?	?	?
Decrease		✓	✓		?	?	?	?

$$\mathrm{SFE} = -4.0 + 2.8 \times \mathrm{Ni(pct)} + 0.39 \times \mathrm{Cr(pct)} + 2.2 \times \mathrm{Mo(pct)} - 2.0 \times \mathrm{Si(pct)} + 0.75 \times \mathrm{Mn(pct)} - 0.47 \times \mathrm{C(pct)} - 12 \times \mathrm{N(pct)}.$$

(Yonezawa 2013)



(Vitos 2006)

❖ Data Mining Approach to SFE

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Current (empirical) model used:

$$\begin{aligned}\mathrm{SFE} = {} & -4.0 + 2.8 \times \mathrm{Ni(pct)} + 0.39 \times \mathrm{Cr(pct)} + 2.2 \\ & \times \mathrm{Mo(pct)} - 2.0 \times \mathrm{Si(pct)} + 0.75 \times \mathrm{Mn(pct)} \\ & - 0.47 \times \mathrm{C(pct)} - 12 \times \mathrm{N(pct)}.\end{aligned}$$

(Yonezawa 2013)

- **Ensure** twin effects through control of stacking fault energy
- Alloy design hinges on **a** proper treatment and interpretation of experimental and theoretical data
- Data mining is great “scaffolding” for **future** alloy design iterations.

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❖ Alumina in Austenitic Steels

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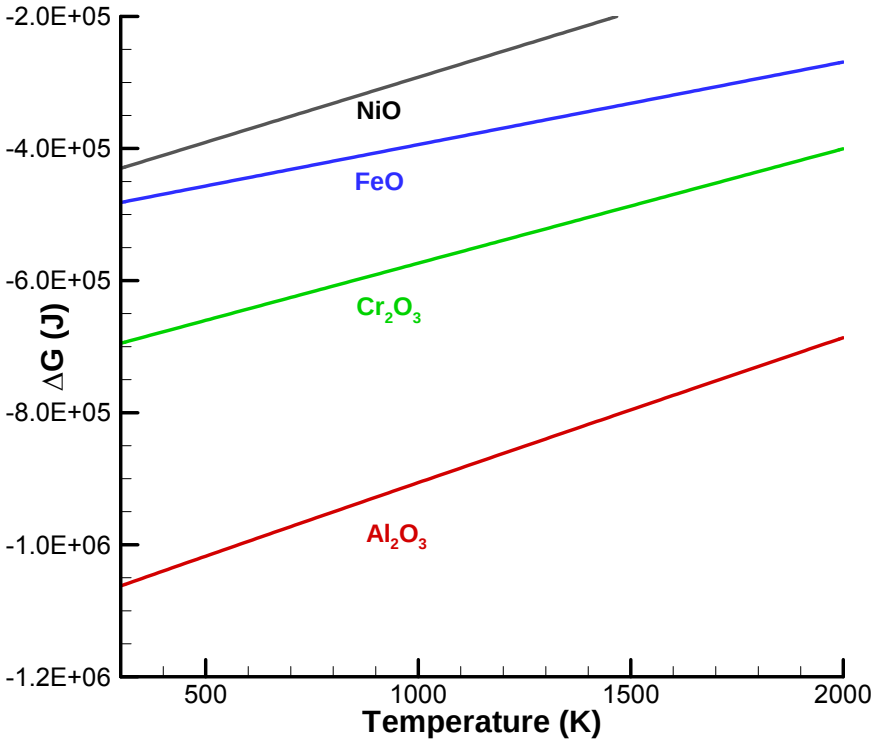
Higher Stability than Conventional Chromium Oxide

- Alumina is also more thermodynamically stable in oxygen than Cr_2O_3 and offers superior protection in many industrially relevant environments.
  - Increased upper temperature oxidation
  - Comparable to more expensive nickel-base alloys
  - Lower cost, formability, and weldability of conventional stainless steels.



Free Energy Stability Comparison

Kubaschewisk O. Met. Thermochem. 1979

Opila EJ. Trans Tech Publ. 2004

Meier GH. Materials and Corrosion 1996

❖ Combined Thermodynamic and Kinetic Criteria: 'effective growth constant'

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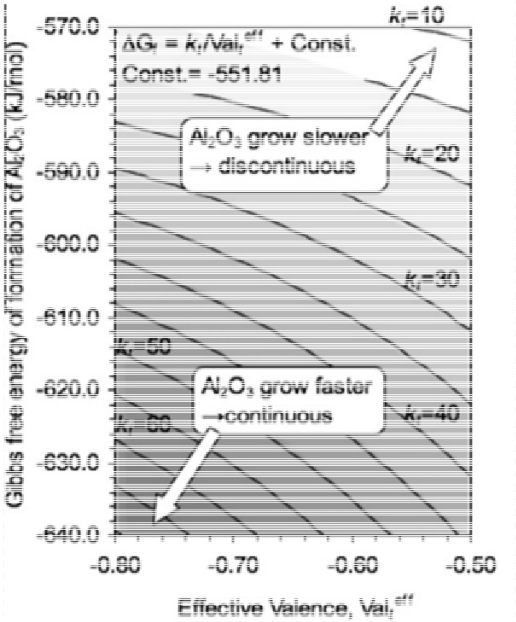
Criteria

For a high chance of establishing a continuous Al_2O_3 layer, the material should have

- High Absolute Effective Valence Value
- High Absolute Gibbs free energy Value
- High K Value



A. Sato et al. Acta Materialia 59 (2011) 225-240

$$\Delta G = \Delta G^0 + RT \ln Q$$

Where

$$\Delta G^0 = 0.2193T - 1127.3137$$

$$Q = \frac{a_{Al_2O_3}^{2/y}}{[a_{Al}]^{2x/y}[P_{O_2}]}$$

$$a_{Al_2O_3}^{2/y} = Unity$$

And

$$Val_t^{eff} \equiv \sum_{n=i} (z_i - z_{al})\bar{c}_i = \Delta e'$$

So

$$\Delta G = (0.2193T - 1127.3137) + RT \ln Q$$

And

$$K \propto Val_t^{eff} \Delta G$$

❖ Testing the 'Effective Growth Constant Criterion'

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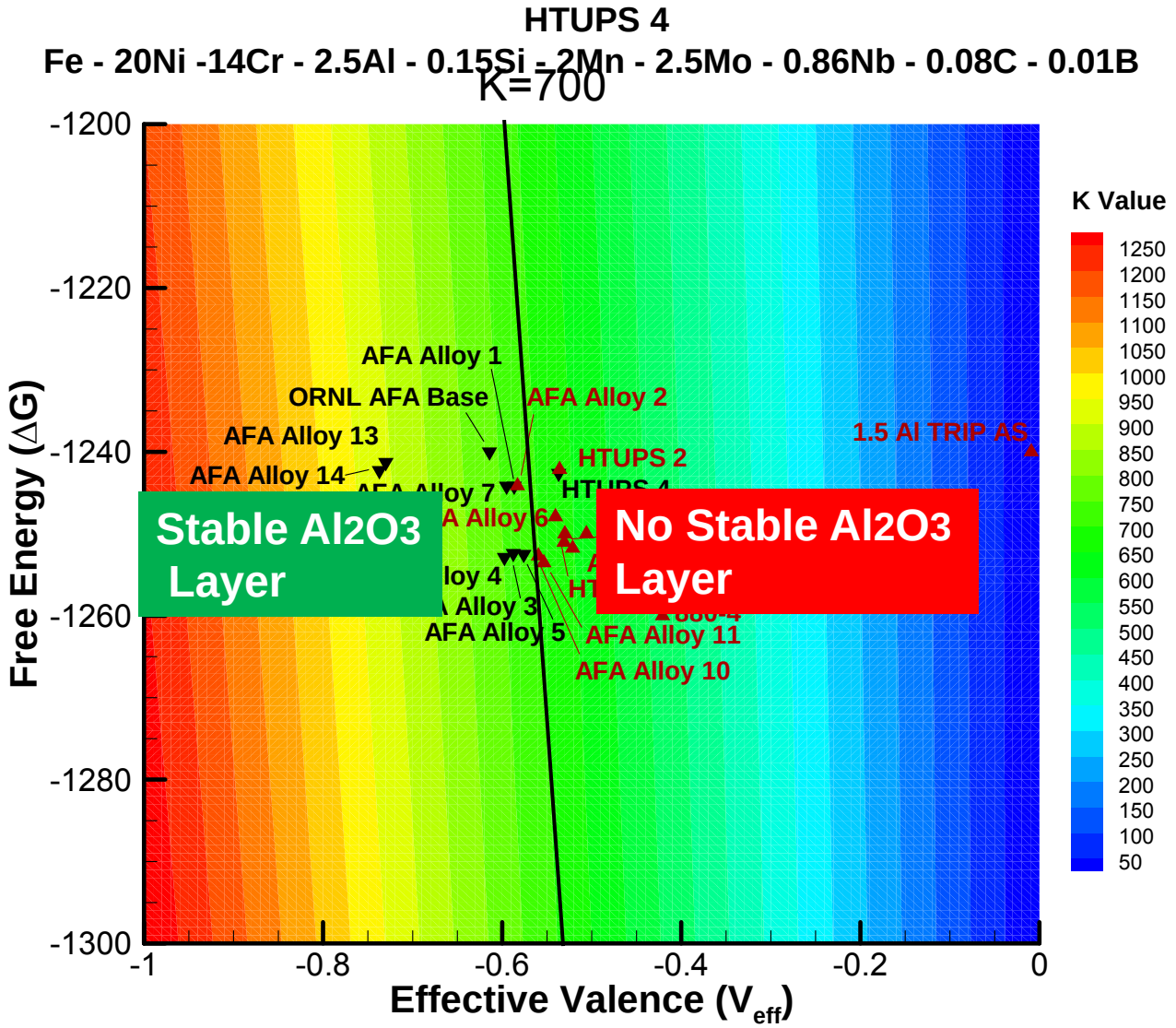

❖ Third Element Effect-Synergies between Chromia and Alumina formation

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$$f_v^* = \frac{N_{Cr}^{O*}\rho(CrO_v)}{F(h_{Cr})} + \frac{N_{Al}^{O*}\rho(AlO_\mu)}{F(h_{Al})}$$

$$N_O^{SO} = G(\gamma)\left[v\frac{N_{Cr}^O}{F(h_{Cr})} + \mu\frac{N_{Al}^O}{F(h_{Al})}\right] \cdot \left[\frac{erf(\gamma) - erf(u_O)}{erf(\gamma)}\right]$$

Where

$$F(r) = \pi^{1/2} r \exp(r^2)[1 - erfc(r)]$$

$$G(r) = \pi^{1/2} r \exp(r^2) erfc(r)$$

And

h_x is defined as $\gamma\varphi_x^{1/2}$ with $\varphi_x = D_O/D_x$

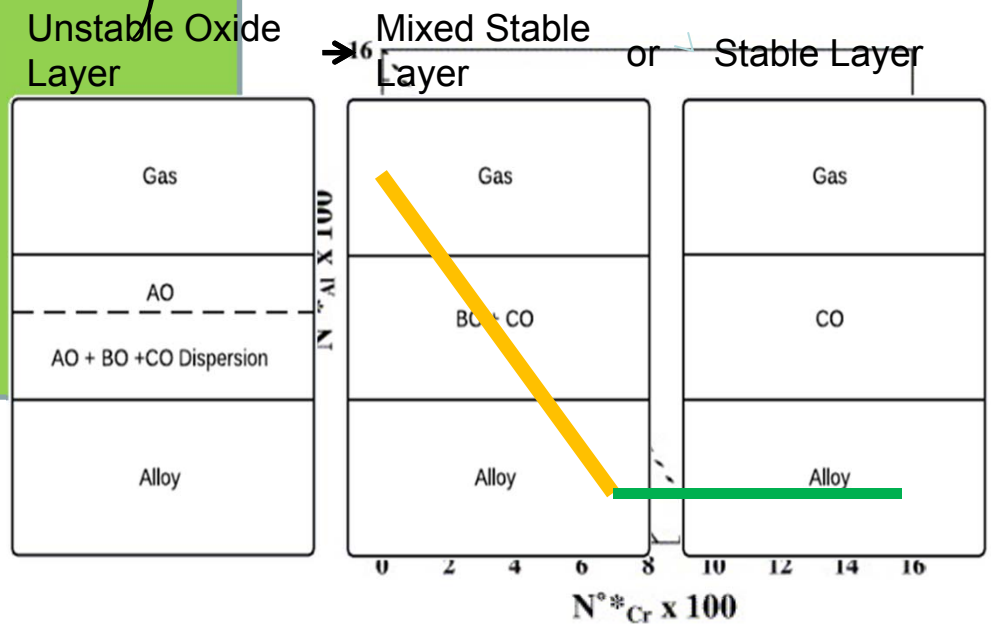
$$N_{Cr}^{O*} = N_{Cr}^{eq}(1 - N_{Cr}^{eq})F\left(\frac{1}{2}[k_c(Cr_2O_3)/D_{Cr}]\right)^{1/2}$$

So

$$N_{Cr}^{O*} = F\left(\frac{1}{2}[k_c(Cr_2O_3)/D_{Cr}]\right)^{1/2}$$

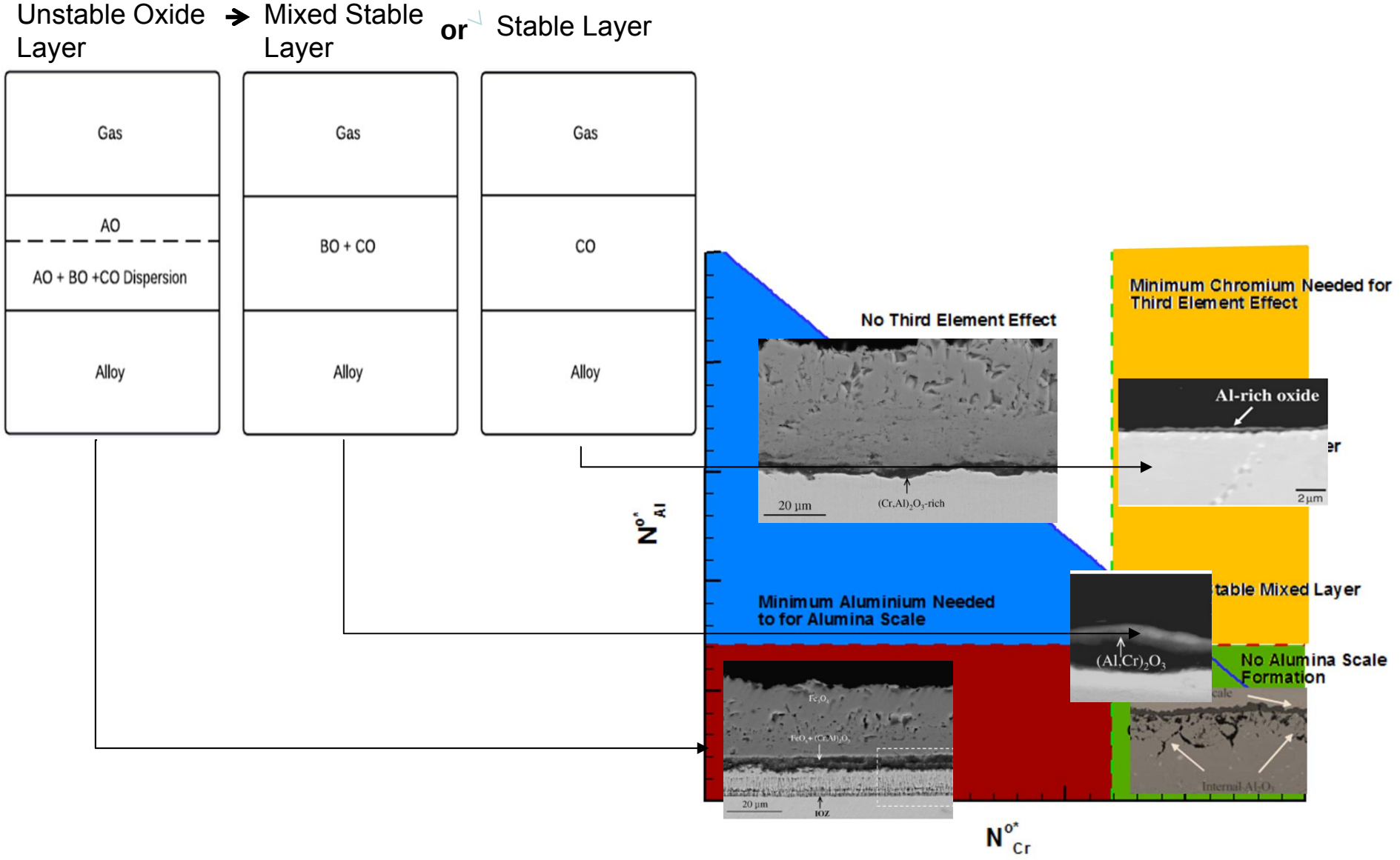
$$N_{Al}^{O*} = F\left(\frac{1}{2}[k_c(Al_2O_3)/D_{Al}]\right)^{1/2}$$

And $N_{Cr}^{eq} << 1$

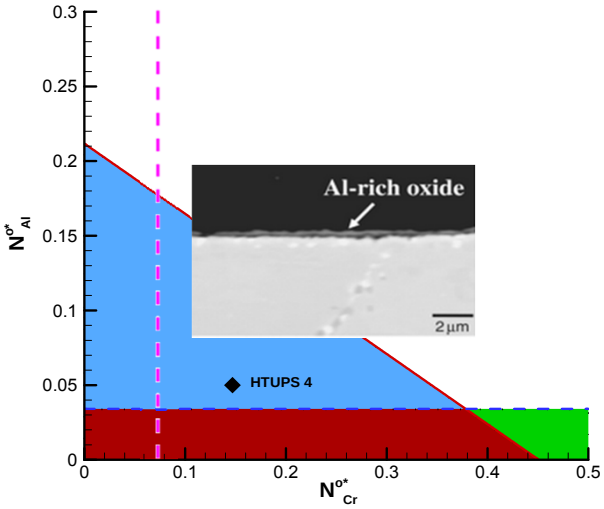


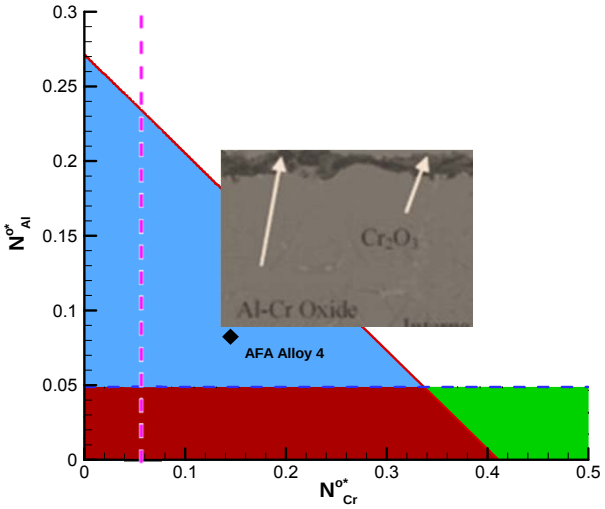
Rapp Robert Corrosion 1965
Niu Y, Gesmundo F. Oxid Met 2004
Crank, John Mathmatics of Diff. 1979
Niu Y, Wang S, Gesmundo F Corr Sci, 2008

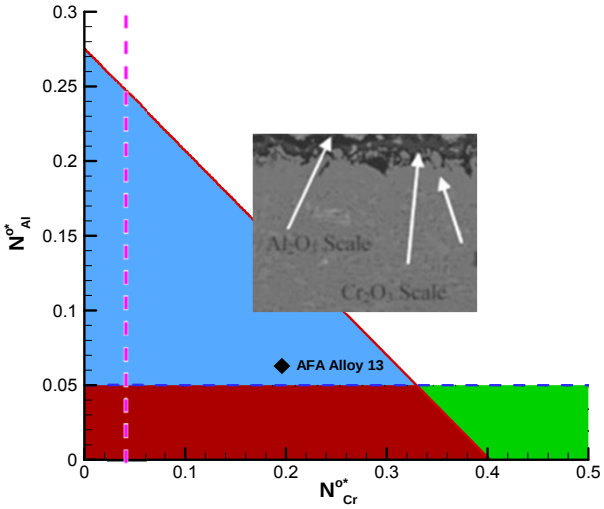
❖ Third Element Effect Predominance Maps



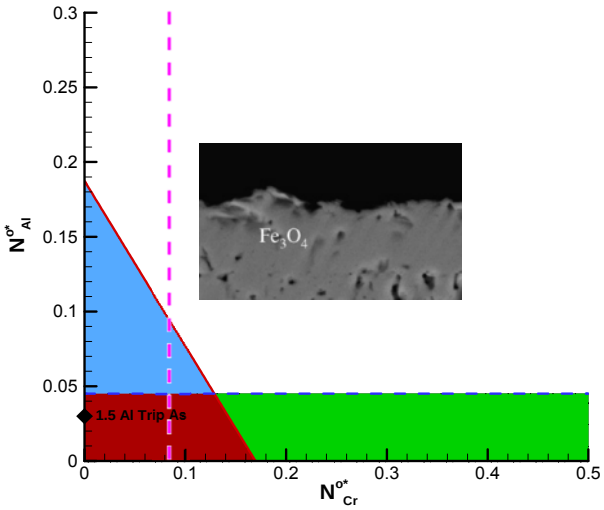
Testing Third Element Effect Predominance Maps

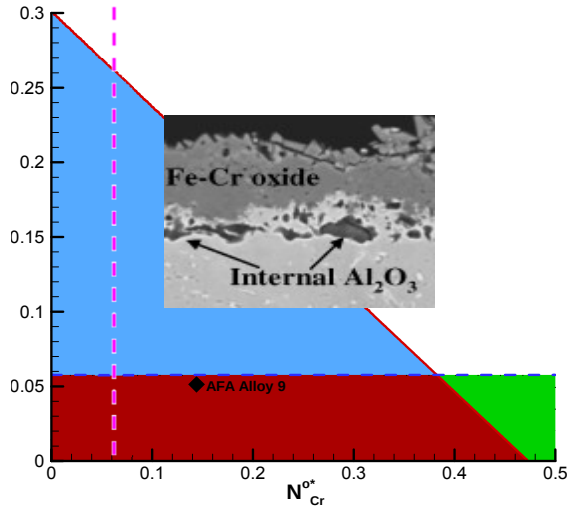


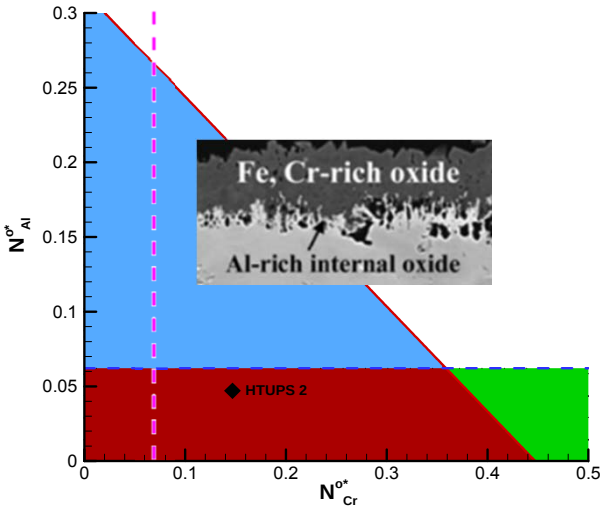




Fe	C	Mn	Si	Cr	Ni	Mo	Cu	W	V	Ti	Al	Nb
Bal.	0.076	1.95	0.15	14.20	20.00	2.46	0.00	0.00	0.50	0.31	2.40	0.14







In This Talk:

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- Experimental determination of stability of deformation twinning nano-structures
- Stacking Fault Energy Models and Data Analysis
- Thermodynamic/Kinetic Criteria for Alumina Formation
- **GA-based Alloy Design**

❖ Genetic Algorithm-based Optimization

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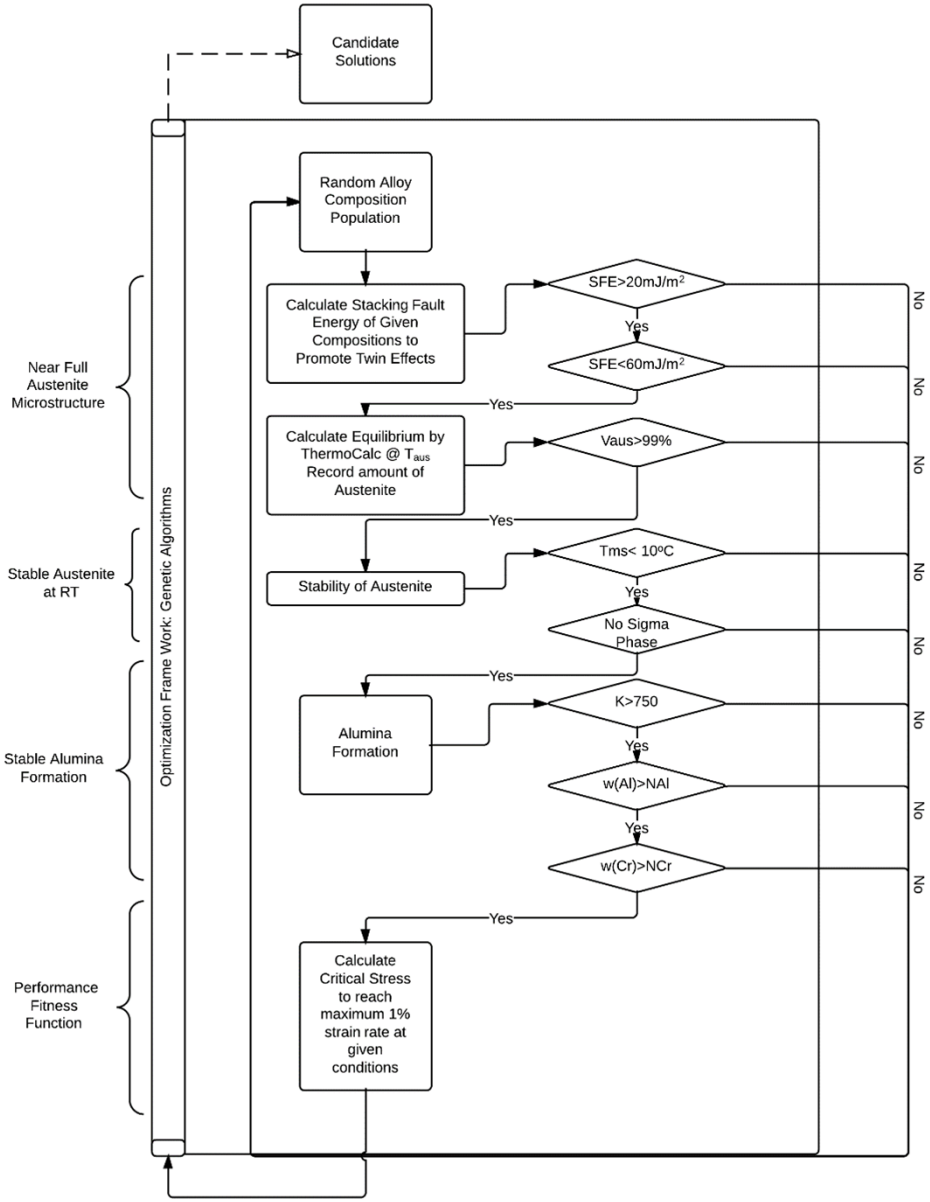
- Computational Genetic Algorithms are a necessity to
  - Streamline Alloy Design Process
  - Decrease Time and Cost of Alloy Discovery
  - Decrease Time and Cost of Alloy Refinement
- GA will be used to find a heat treatment process for
  - Maximizing FCC Phase
  - Minimize BCC and Unwanted Phases
  - Ensure Twinnability through control of Stacking Fault Energy
  - Austenite Stability
  - Alumina Formation
  - Critical Stress for Creep



❖ Proposed Genetic Algorithm Alloys

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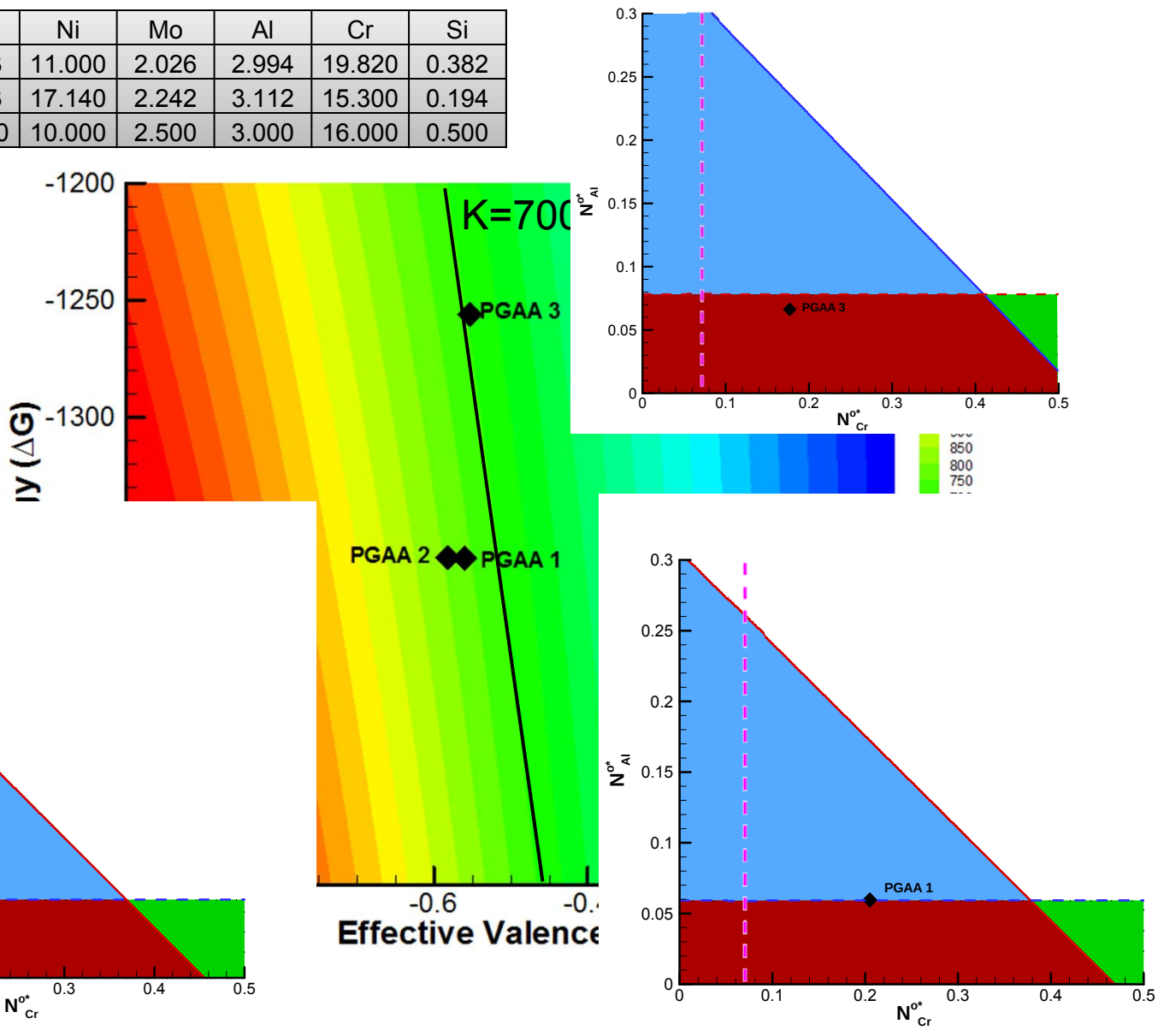
PGAA	Fe	C	Mn	Ni	Mo	Al	Cr	Si
1	Bal.	0.073	3.893	11.000	2.026	2.994	19.820	0.382
2	Bal.	0.088	8.993	17.140	2.242	3.112	15.300	0.194
3	Bal.	0.050	10.000	10.000	2.500	3.000	16.000	0.500



Future Plans

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- Formulate twinnable, alumina-forming composition
  - Difficult problem: Al increases SFE, low Al reduces stability of alumina layer. Must lower SFE through alloying
- Investigate thermal stability of deformation twins
  - We know we can design alloys that exhibit significant nano-structured deformation twins.
  - Twins appear to be stable in the short term. What about long-term stability?
  - What is the effect of twin structure on ReX?

Future Plans, ctd

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- Investigate effect of nano-precipitates
  - How do nano-precipitates interact with twins?
- Comprehensive Alloy Optimization:
  - Alumina, twinnability, nano-precipitates
  - Prepare alloys, characterize mechanical response, long-term behavior

Backup slides

❖ Approach

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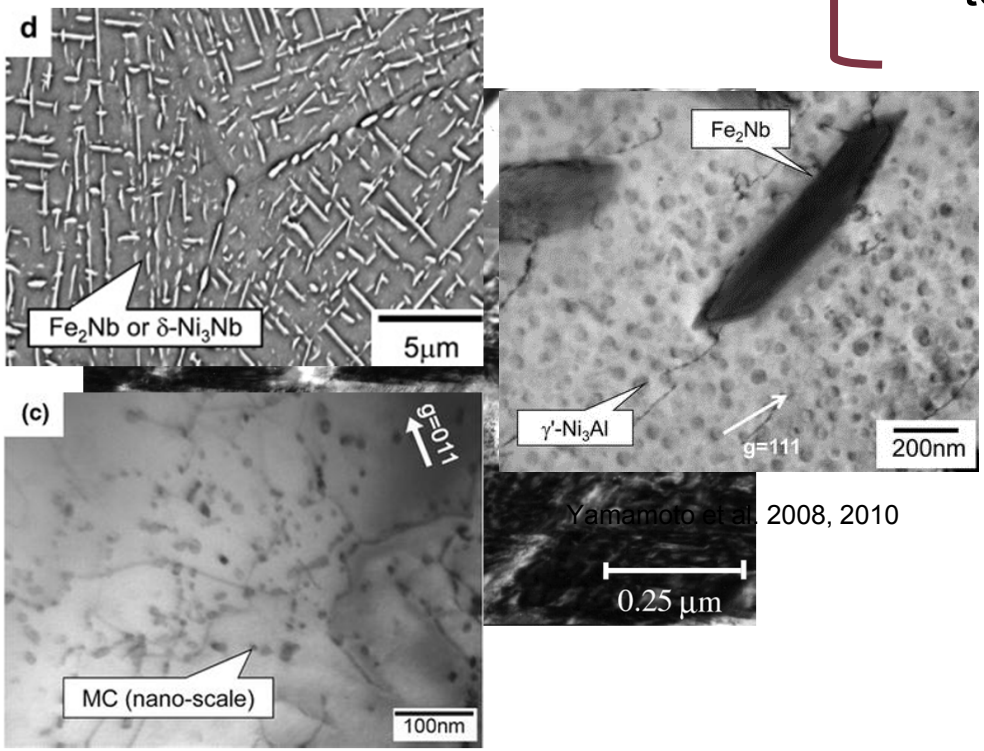
Alloy + Microstructure Design

- Austenitic structure
- High density of low energy grain boundaries or nano-twin boundaries
- Nano-scale precipitates, intermetallics, laves phases stable at high temperature



Yamamoto et al. 2008, 2010

❖ Approach

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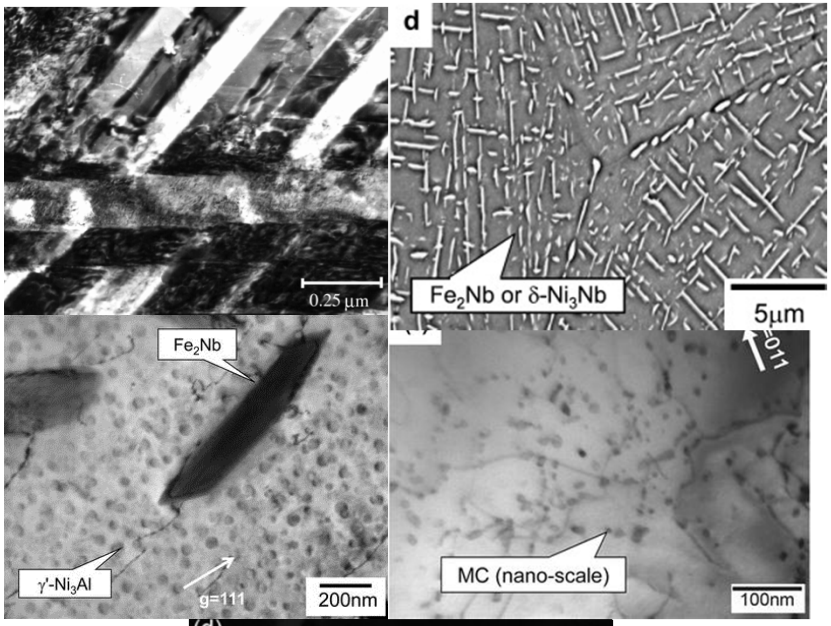
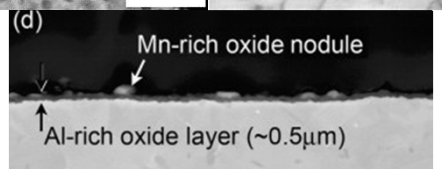
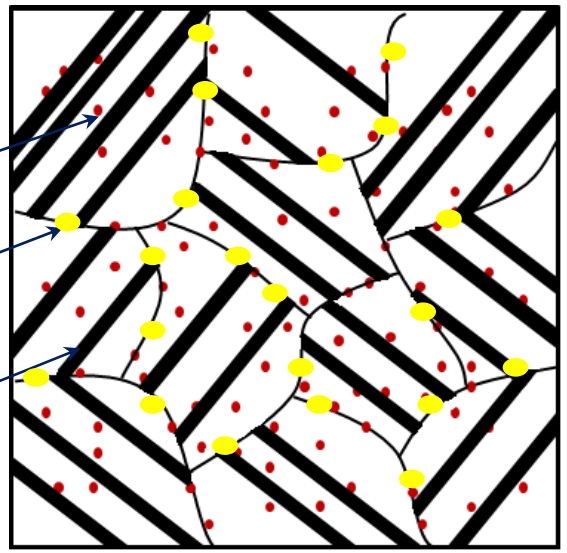
Alloy + Microstructure Design

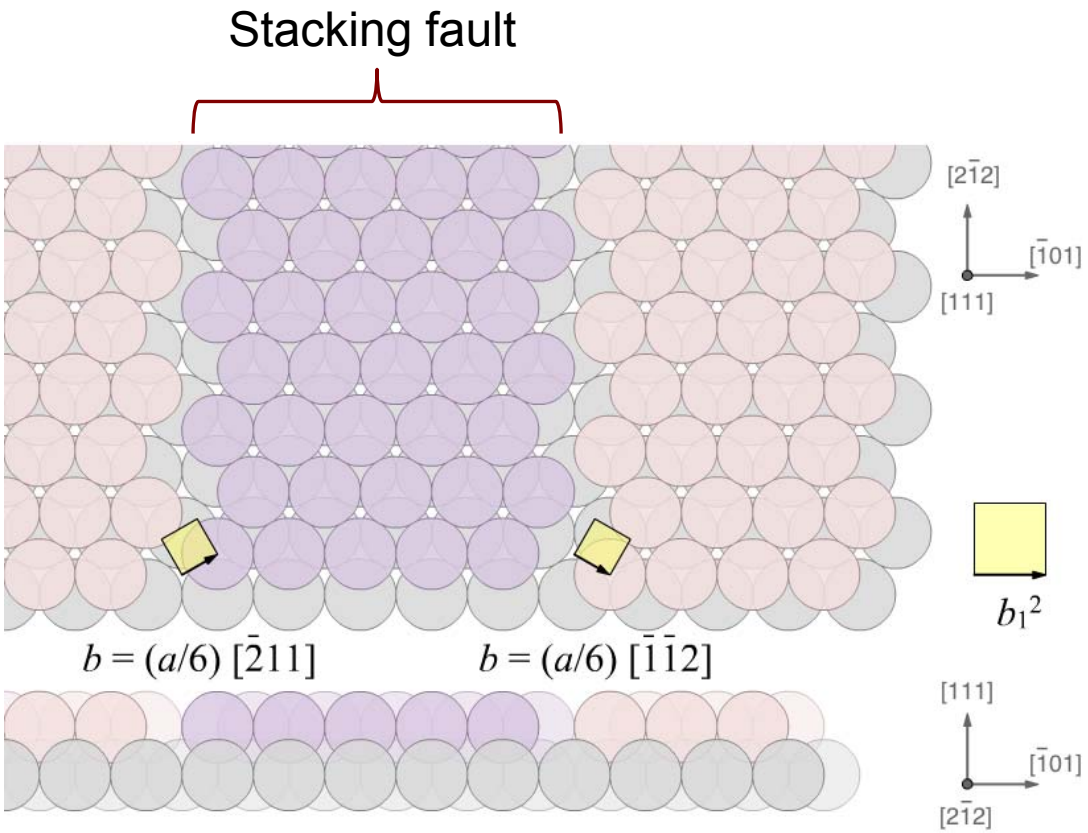
- Austenitic structure
- High density of low energy grain boundaries or nano-twin boundaries
- Nano-scale precipitates, intermetallics, laves phases stable at high temperature
- Formation of alumina surface oxide



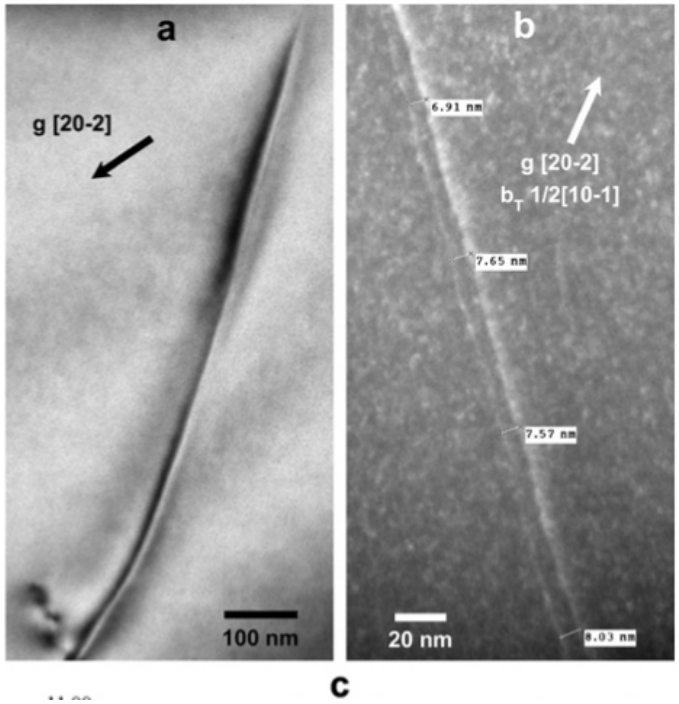




❖ Stacking Fault Energy



Dissociated unit dislocation



BF WBDF

TEM spacing measurements

(Pierce 2012)

❖ Measuring SFE

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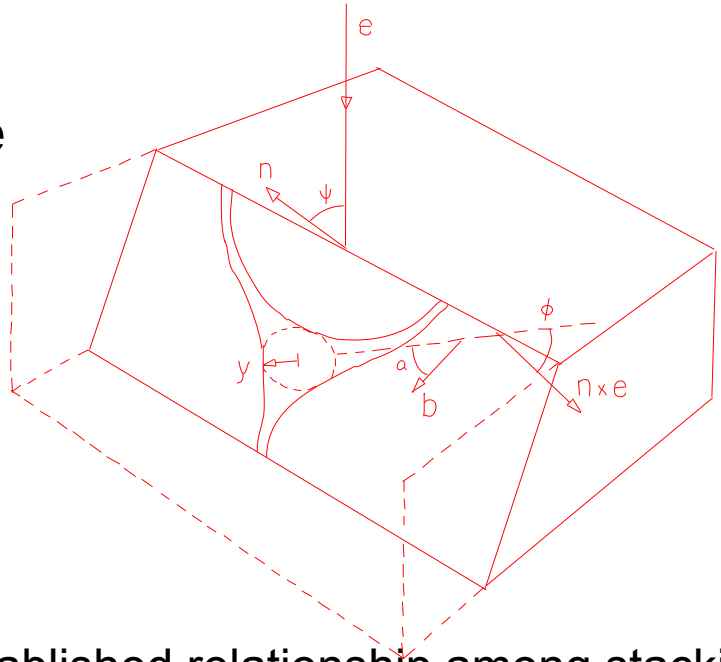
Transmission Electron Microscope

- Direct observation of faulted dislocation structures
  - Dislocation nodes
  - Multiple ribbons
  - Stacking fault tetrahedral
  - Faulted dipoles



X-ray Diffraction

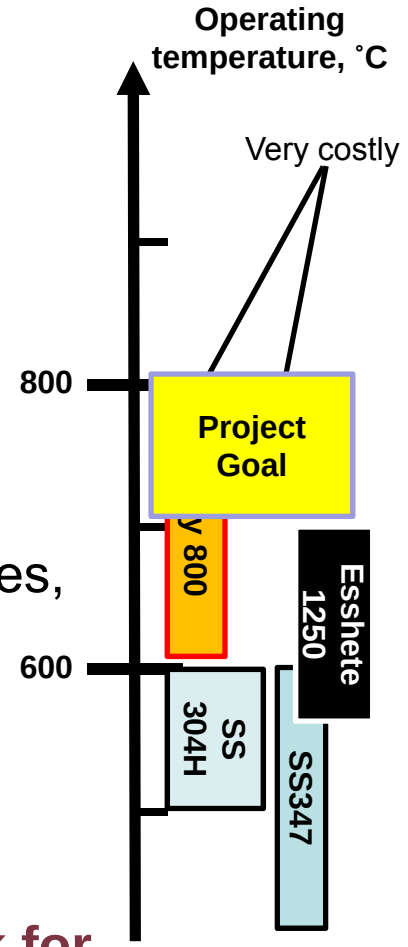
- Research by Reed and Schramm- established relationship among stacking fault probability and microstrain
  - Stacking faults affect XRD line shift and line broadening
  - In-situ XRD: SFE determined from critical shear stress (David Rafaja, 2013)

Others:

- **HREM, Texture, Creep**

❖ Project Goals

- Design new austenitic stainless steels (ASS) for advanced ultra supercritical combustion coal-fired power systems
  - ✓ High temperature strength
  - ✓ High ductility
  - ✓ Good creep resistance
  - ✓ Good high temperature oxidation/corrosion resistance
- Design of micro-alloying additions, heat treatment schedules, and microstructure
  - Cost-effective alternatives to Ni-base superalloys
  - Higher-temperature alternatives to ferritic steels
- **Develop a robust ICME design/optimization framework for high temperature ASS.**



❖ Thermodynamics of Oxide Layer Formation

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4 Al + 3 O_2 ➡ 2 Al_2O_3

4 Cr + 3 O_2 ➡ 2 Cr_2O_3

$$\Delta G = \Delta G^0 + RT \ln Q$$

At equilibrium

$$\Delta G = 0, Q = K_c$$

$$\Delta G^0 = -RT \ln K_c$$

So

$$\Delta G = -RT \ln K + RT \ln Q$$

$$\Delta G = RT \ln \frac{Q}{K_c}$$

Where

$$K_c = \exp\left(\frac{-\Delta G^0}{RT}\right) \quad Q = \frac{a_{Al_2O_3}}{[a_{Al}]^2[a_O]^3}$$

If $K_c > Q$ *then forward reaction*
If $K_c < Q$ *then backward reaction*

C.H.P. Lupis Chemical Thermodynamics of Materials