SAND2016-10004C

Dependence of Grain Boundary Structure on Radiation Induced Segregation and Void Denuded Zones in a Model Ni-Cr Alloy

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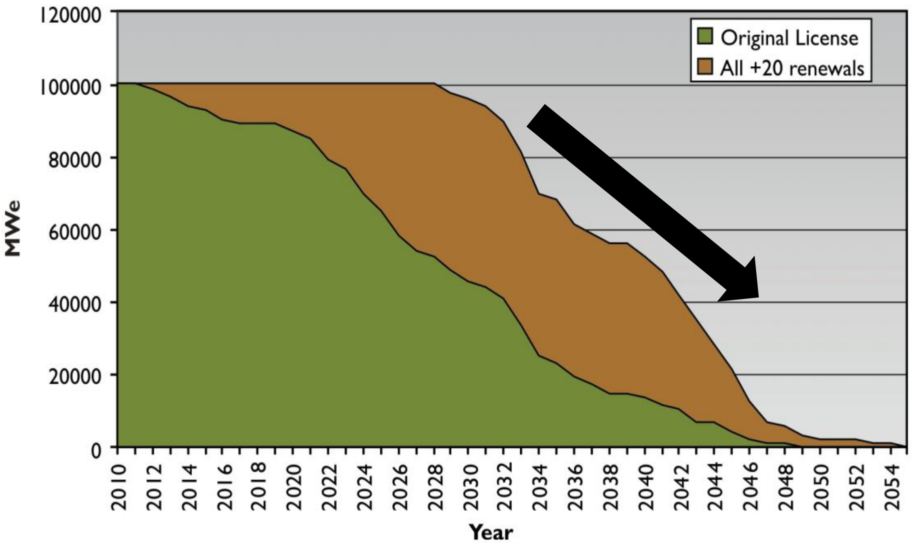
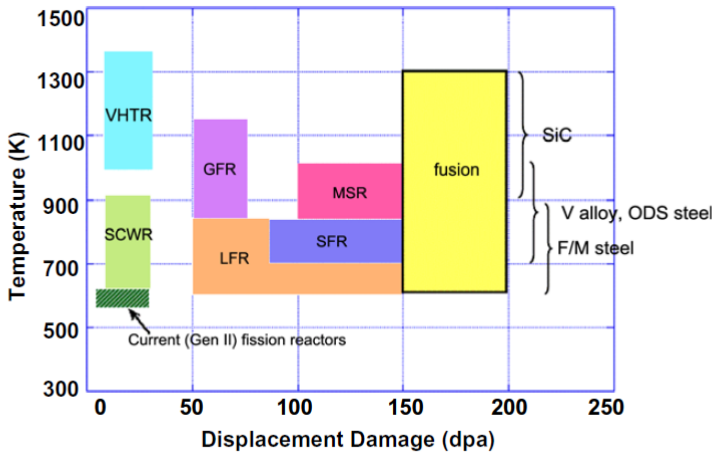
Motivation: Aging Reactors and Materials Failure

- Key non-fossil fuel energy system for electrical demand in emerging and existing markets
- Safe and reliable material extension for current LWR materials and future nuclear reactor designs
- Ageing fleet, average age is > 35 years: high maintenance and upgrade cost
- **Next generation → new alloy development**

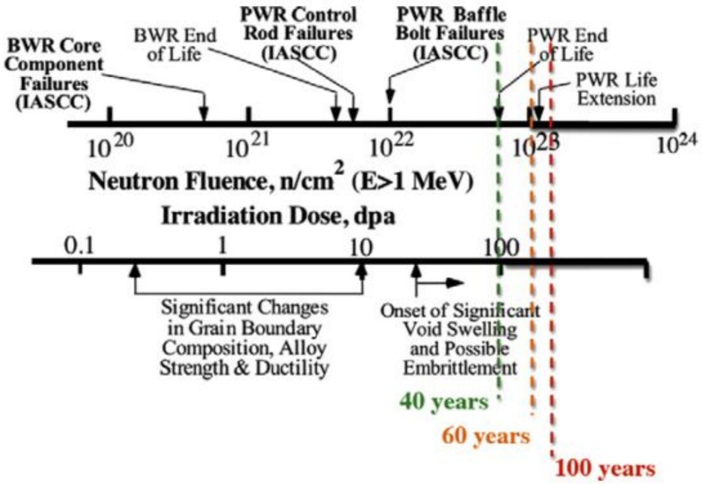
Estimated energy output from existing reactors



US-DOE Report to congress, 2012



Yvon and Carré, JNM (2009)



Was and Zinkle, Acta Mat. (2013)

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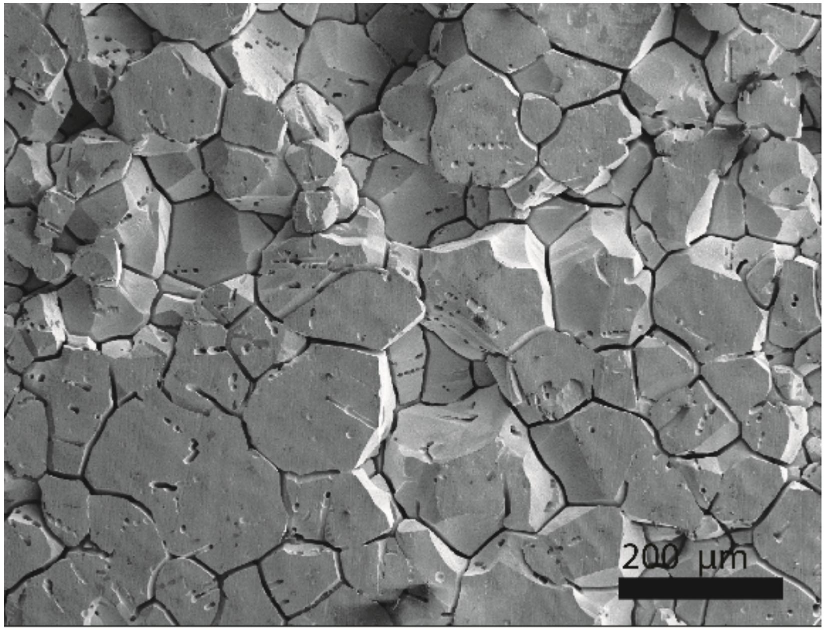
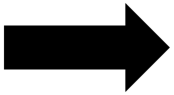
Tailored Microstructures for Extreme Environments

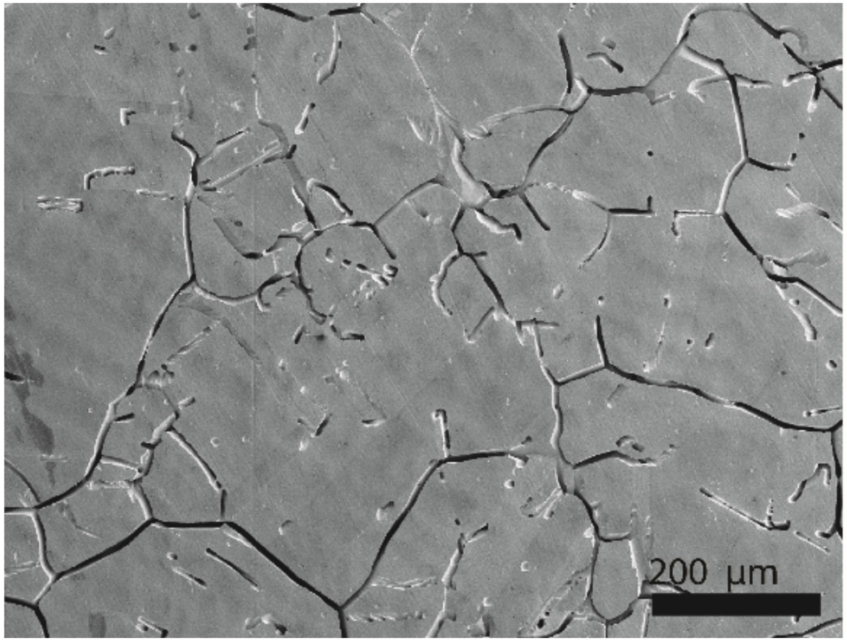
- Grain boundaries (GBs) are a critical material interfaces → tailoring network provides method for sophisticated microstructures
- **GB character** → variations in GB structure/properties can lead to subsequent changes in response to extreme environments

Standard 316: 4.2 mm/yr.





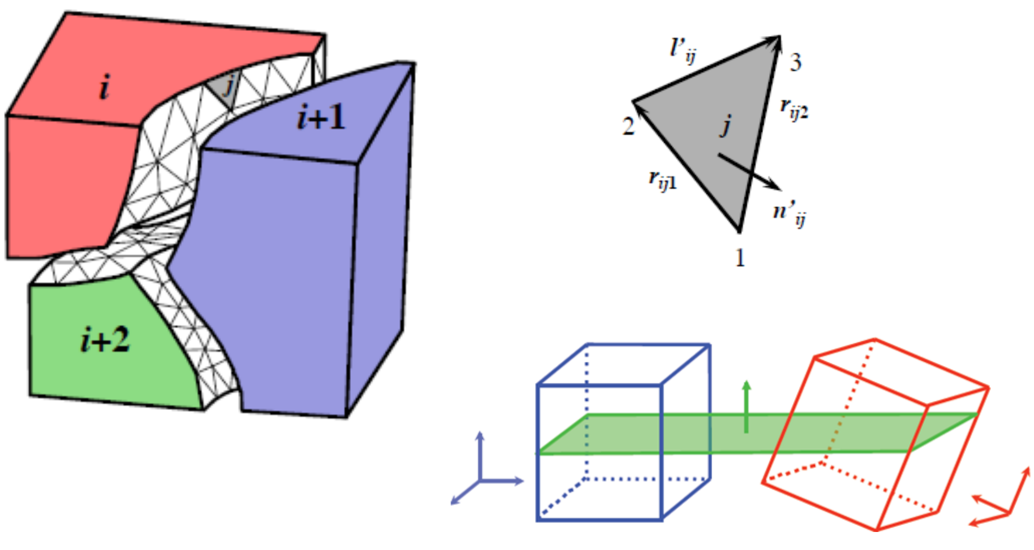
Engineered 316L: 2.2 mm/yr.



Barr et al. Corrosion Science (2016), under review

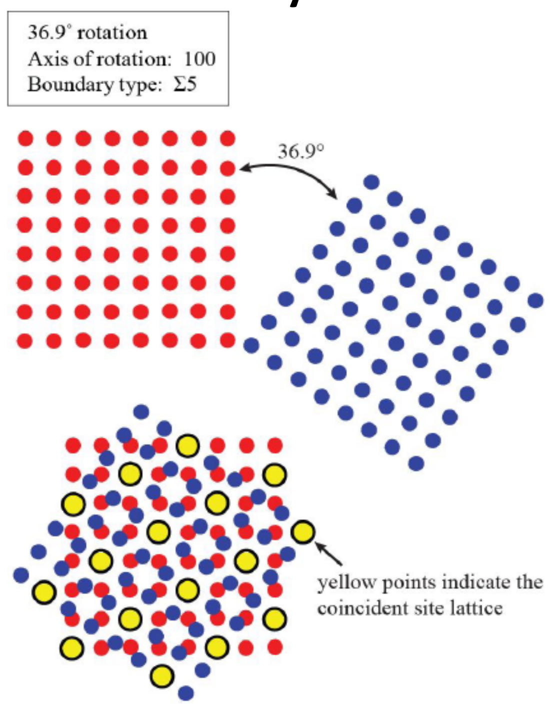
Background: Grain Boundary Structures

- High and low angle GBs, tilt/twist, symmetric/ asymmetric
- Coincidence Site Lattice (CSL) notation (geometric model)
- Reports indicate a link between some CSL GBs (e.g. Σ3) and improvements in intergranular corrosion, stress corrosion cracking, and hydrogen embrittlement



Misorientation (Δg) and grain boundary plane normal (**n**)

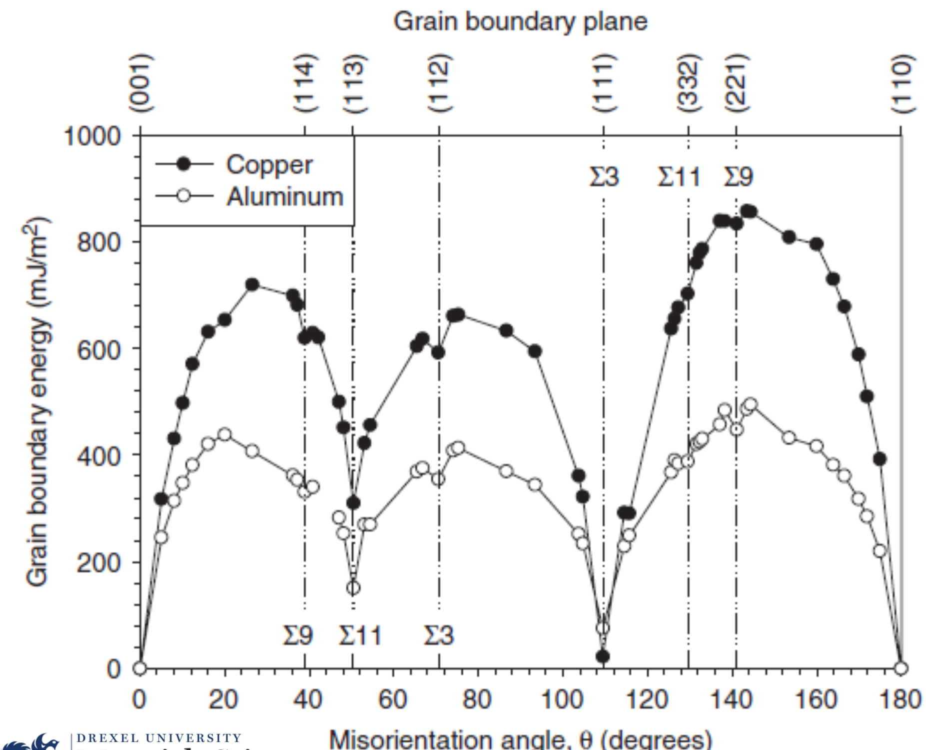
CSL Boundary Notation



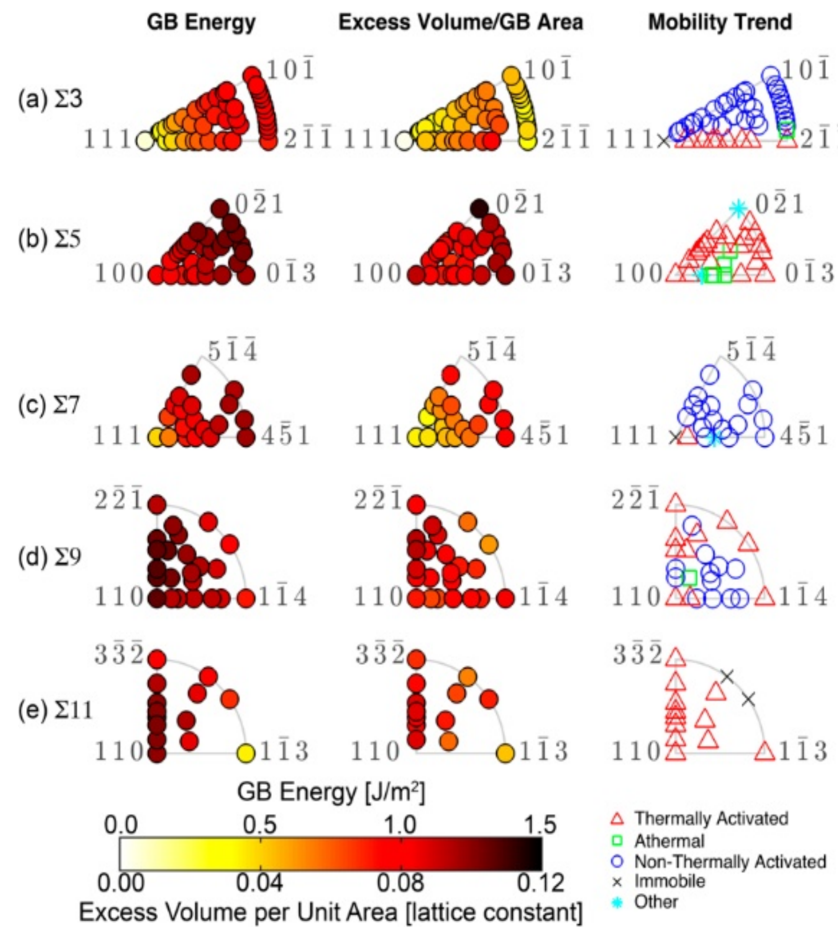
E.A. West, Michigan (2010)

GB Structure – Property Relationship

- GB landscape highlights specific GBs that have low energy or excess volume
- GB energy does not correlate with “low” coincidence site lattice (CSL) Σ GBs
- GB-defect interactions: formation energies, load/pristine GBs, interaction widths



Tschopp et al., Phil Mag (2009)



Homer et al., Sci. Reports (2015)

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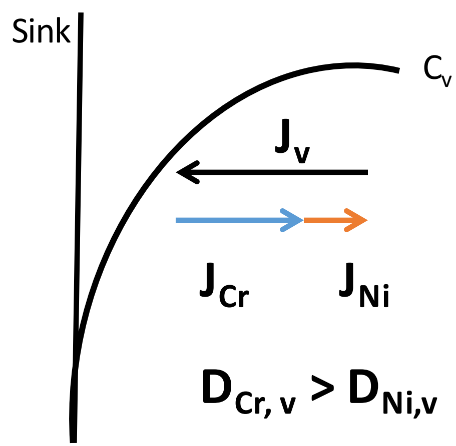
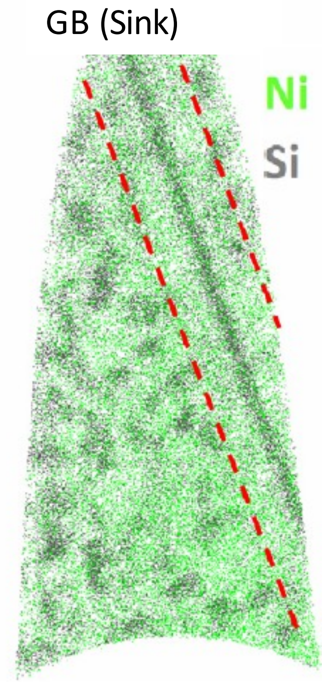
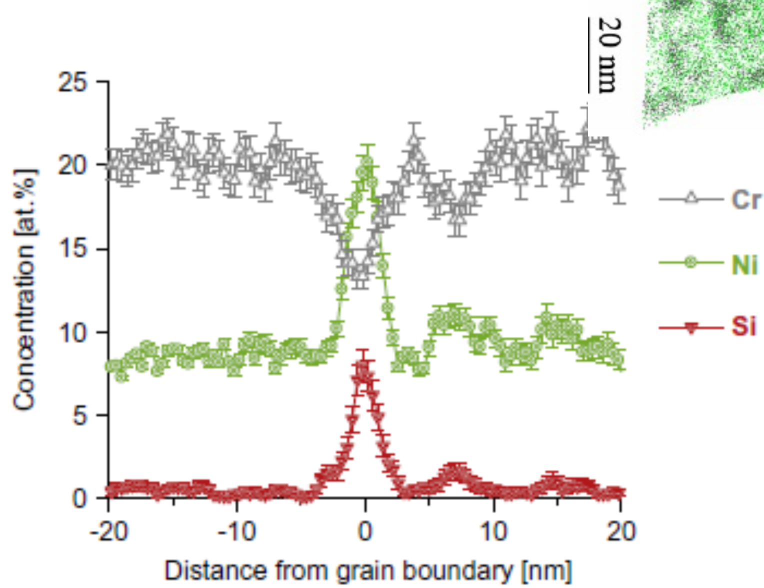
Radiation Induced segregation (RIS):

- Non-equilibrium segregation of alloying elements caused by flux of irradiation induced defects
- Alloying elements segregate when a specific species is preferentially interacting with a defect flux
- **Vacancy-species preferential interaction**
  - **Vacancy-solute exchange mechanism**
- Interstitial-solute exchange mechanisms

Model Binary alloy with vacancy dominated RIS







T. Toyama, et al., JNM, 2012   Jiao et al. Acta Mat. (2011)

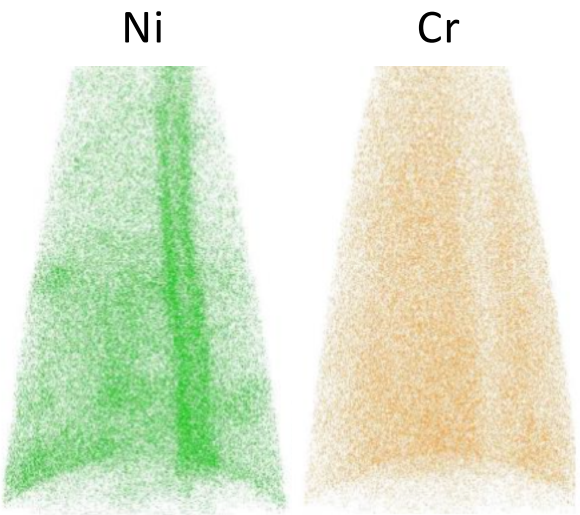
Objective:

Project Goals:

1) Design microstructure capable of obtaining particular improvement in irradiation response through GB character evolution

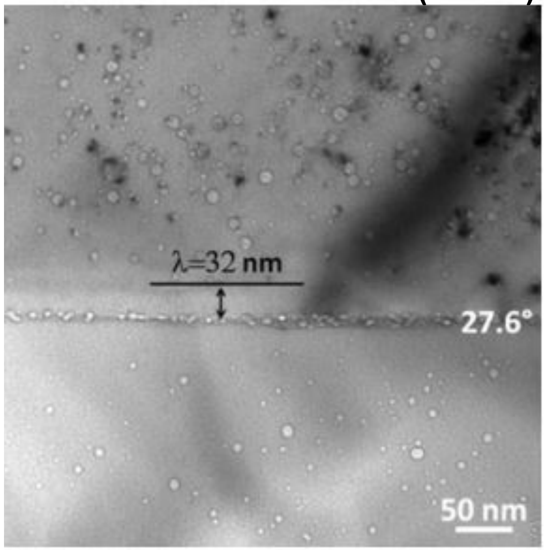
2) Provide predictive understanding of how particular GB structures respond under radiation induced segregation and void denuded zones.

Two Case Studies: Engineering Alloy 316 and Model Ni-Cr Alloy



Barr et al., submitted JNM (2016)

Void denuded zones (VDZs):



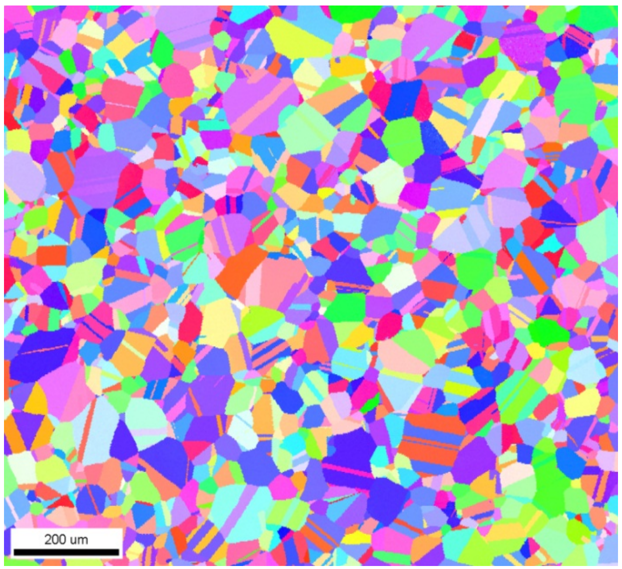
Han et al., Acta (2012)

Grain Boundary Engineering (GBE) in 316L:

- GBE structure → design of experiment with different strain, time, and temperature

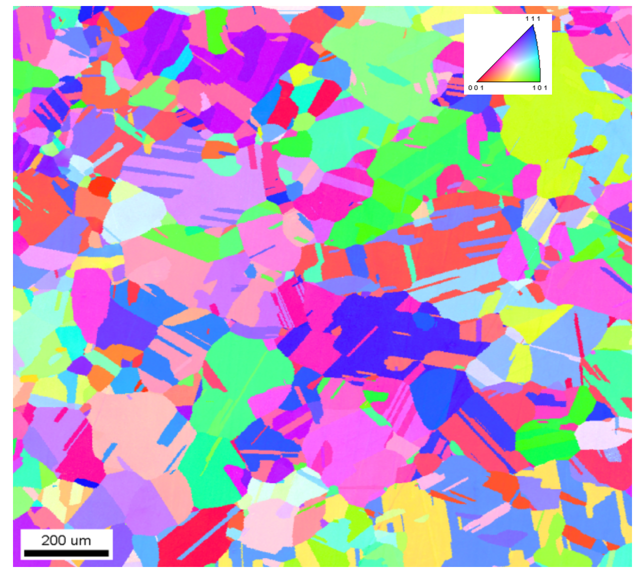
Alloy	Fe	C	Mn	P	Si	Ni	Cr	Mo	Cu
wt. %	Bal	0.02	2.0	0.02	0.3	14.7	17.5	2.8	0.1

Solution Anneal:



GBE Processing →

GBE: 5% RR-1000˚C-60 minutes



GB Population Statistics — Triple Junction Distribution (TJD)

	Σ3	Σ9+Σ27a,b	Σ3n	HV	Grain dia (µm)	TJD: Σ3c-Σ3c-Σ9	TJD: Σ3c-R-R	TJD: Σ3i-Σ3c-Σ9
Sol Anneal	47	0.9	47.9	150	47	2.6	50.9	1.1
GBE	68.2	8.9	77	143	100	9.5	32.5	10.1

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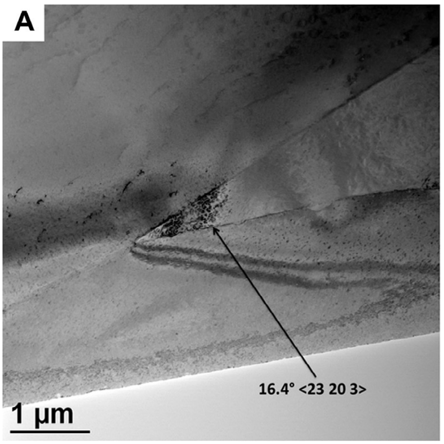
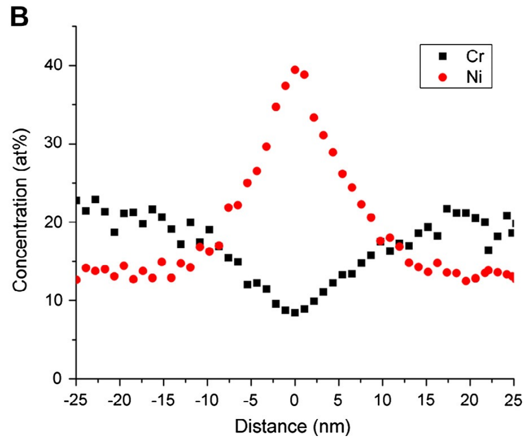
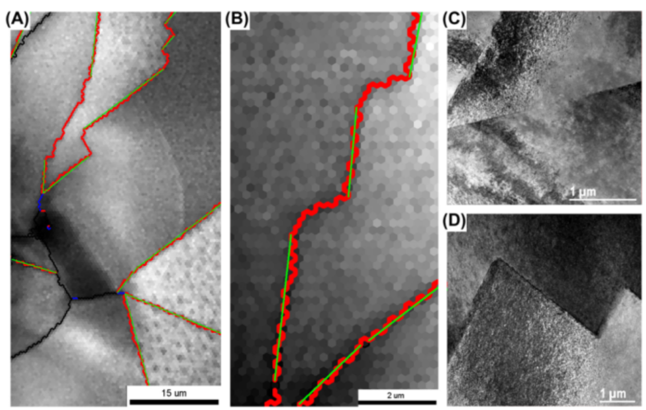
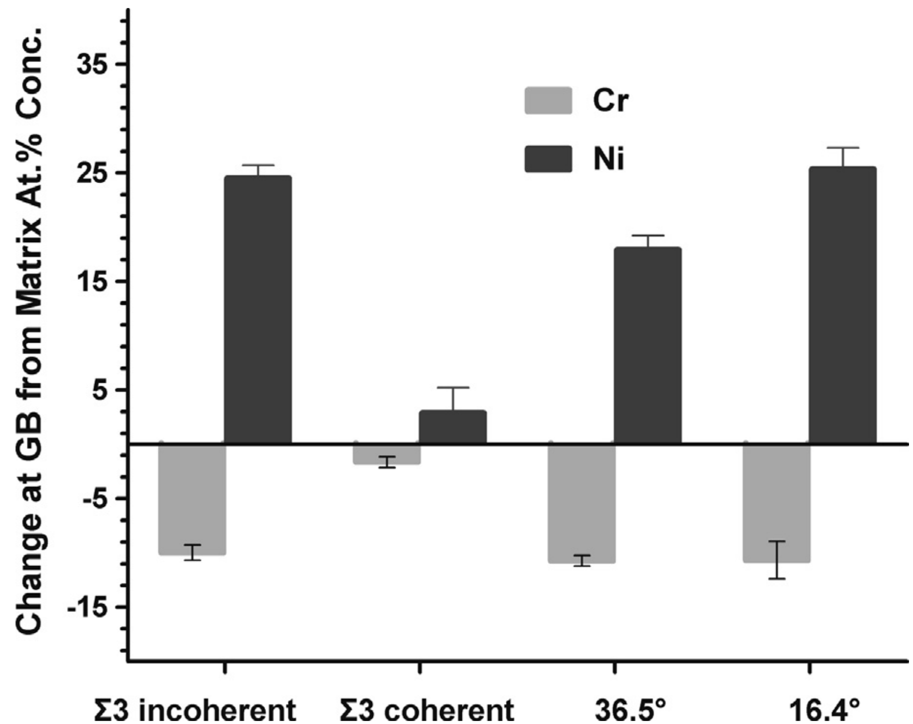
C.Barr et al., Corrosion Science, under review (2016)

Grain Boundary Dependent RIS in 316L:









- 11 dpa, 1.6×10^{16} ions cm^{-2}, 3 MeV Cu^{2+} heavy ion irradiation, 500˚C
- Strong dependence on grain boundary coherency
- Minimal Cr depletion variation observed between random HAGB types

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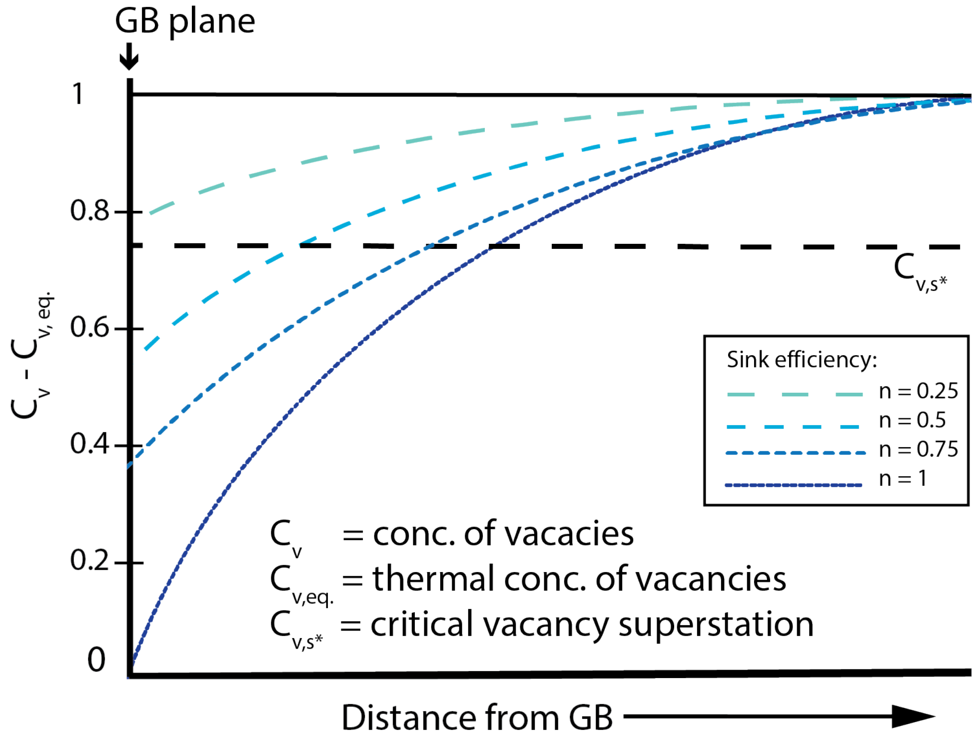
C.M. Barr et al. Acta Materialia 67 (2014): 145-155

Model Ni-Cr Alloy:

Simple binary alloy provides more direct comparison to models

→ Correlated model-experiments provide ideal approach for predictive microstructural evolution under irradiation

- Variations in the radiation response should exist as function of GB character and subsequently have **different sink efficiency** dependent upon:
  GB energy/free volume: misorientation + inclination

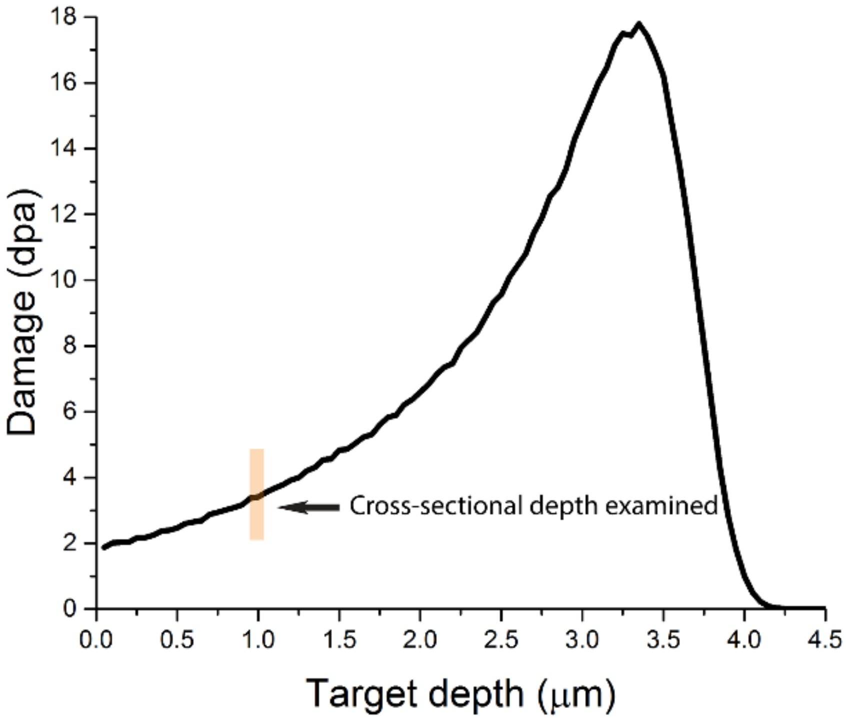


Experimental Methods – Ion Beam Irradiations:

- Thermomechanical processing used to induced wide range of available GBs
- 20 MeV Ni^{4+} at 500°C on bulk Ni-5Cr to 3.4 dpa at 1um depth
- SRIM used to calculate dpa using Kinchin-Pease method with quick cascade based

Heater and sample for bulk irradiations:

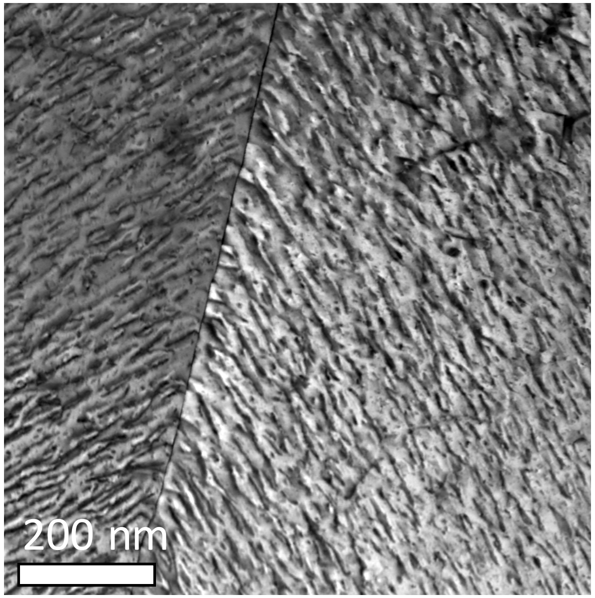
SRIM determined damage profile for sample cross-sectional



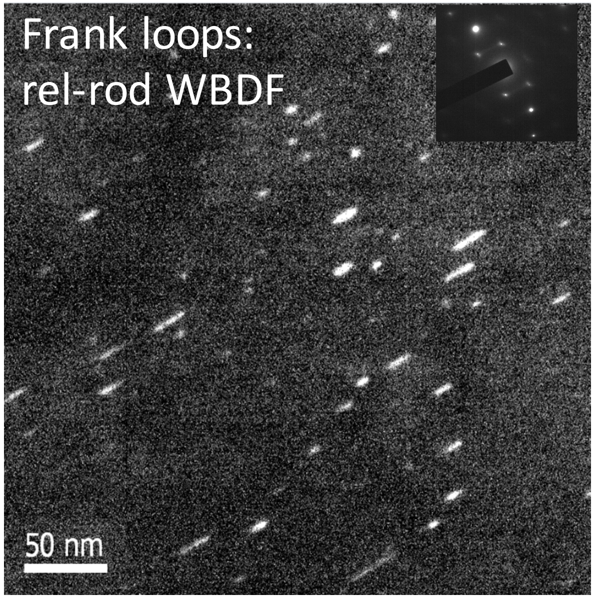
GB Character Irradiation – Defect Size Distribution:

- 1.9 x 10^{16} ions/cm^2
- 3.4 dpa at 1 µm depth
- Avoided injected interstitial effects at examined cross-sectional depth

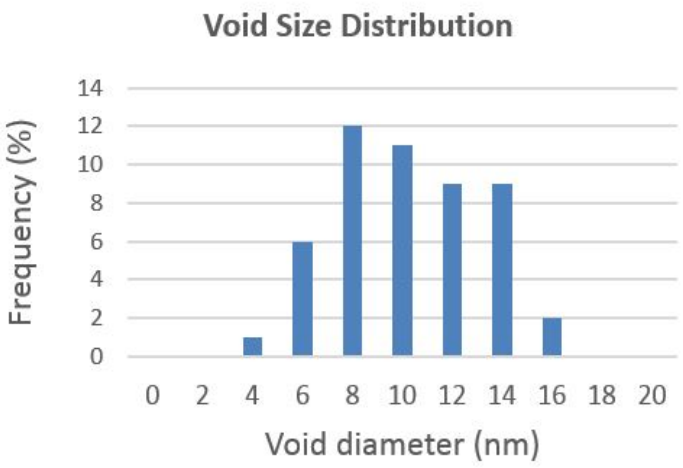
BF-STEM:



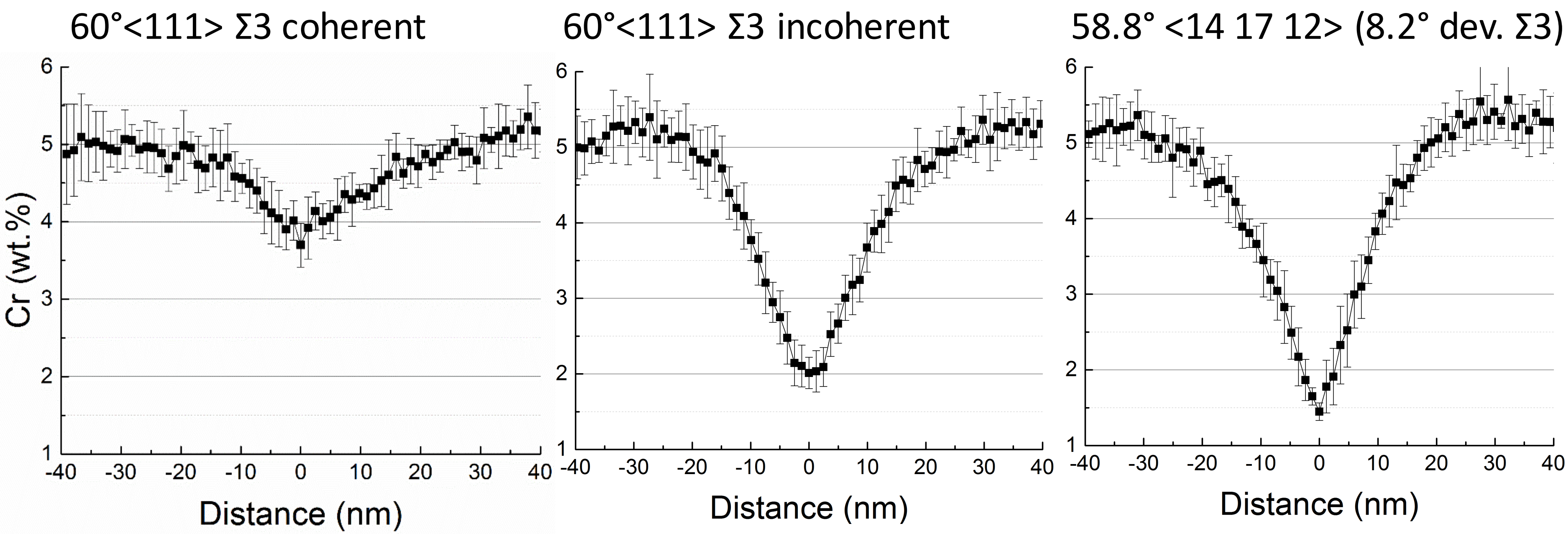
Defect density: 1.16x10^{22} m^{-3}



Void density = 9.09 X 10^{20} m^{-3}



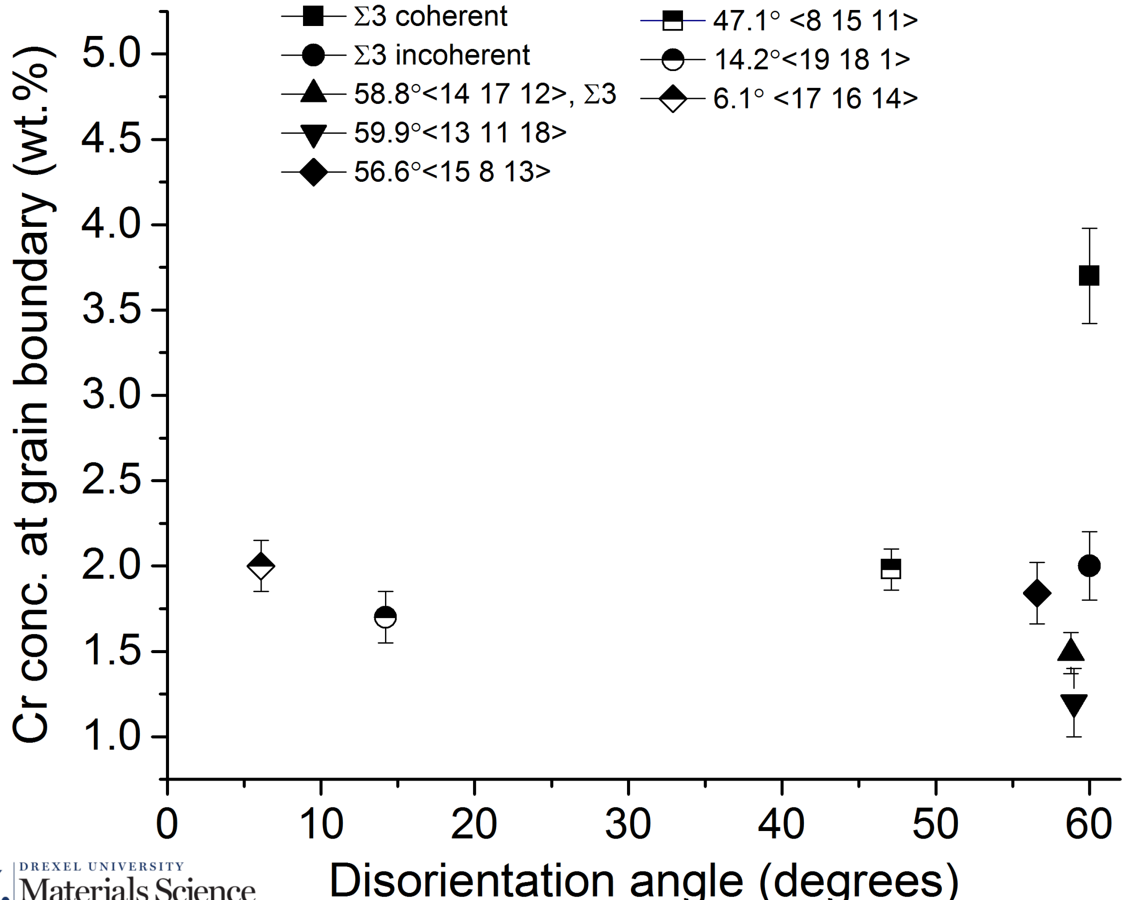
GB Character Irradiation – Σ3 RIS:

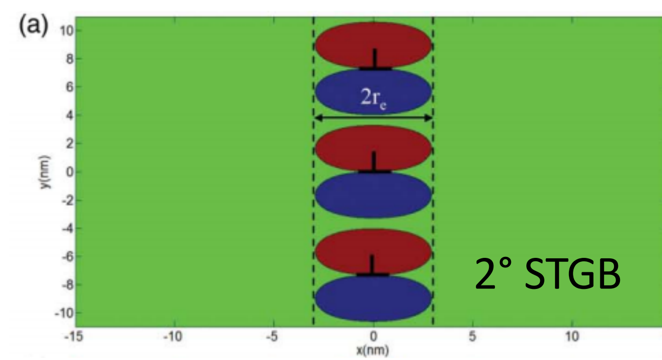


- Heavily anisotropic RIS within GBs considered "Σ3"
- Clear distinction and response between coherent and incoherent twins
- Sink efficiency low for coherent plane {111} twin compared to incoherent plane {112}
- 58.8° heavily deviated Σ3 behaves like random HAGB

GB Character Irradiation – Low and High Angle GBs:

- No statistical different between RIS response at high and low angle GBs
- RIS measured at a ~3.4 dpa in steady-state irradiation regime
- Possible reason for the absence of the expected reduction in sink efficiency for low GB angles are GB strain effects

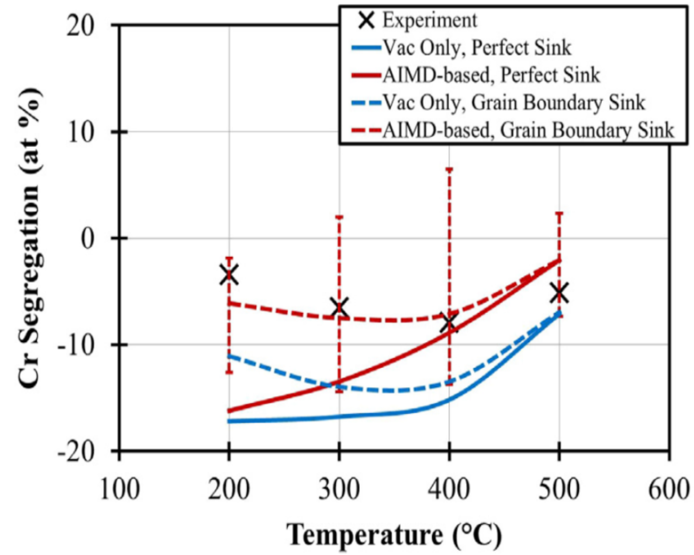




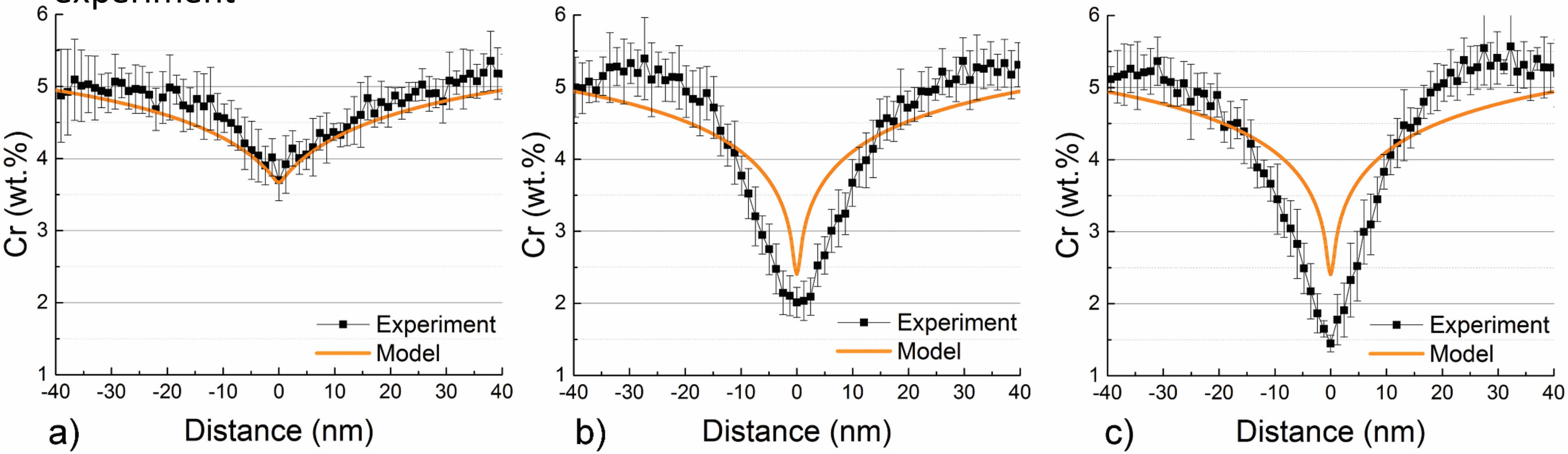
Jiang et al., MRL, **2**, (2014)

GB Character Irradiation – RIS Model Comparison

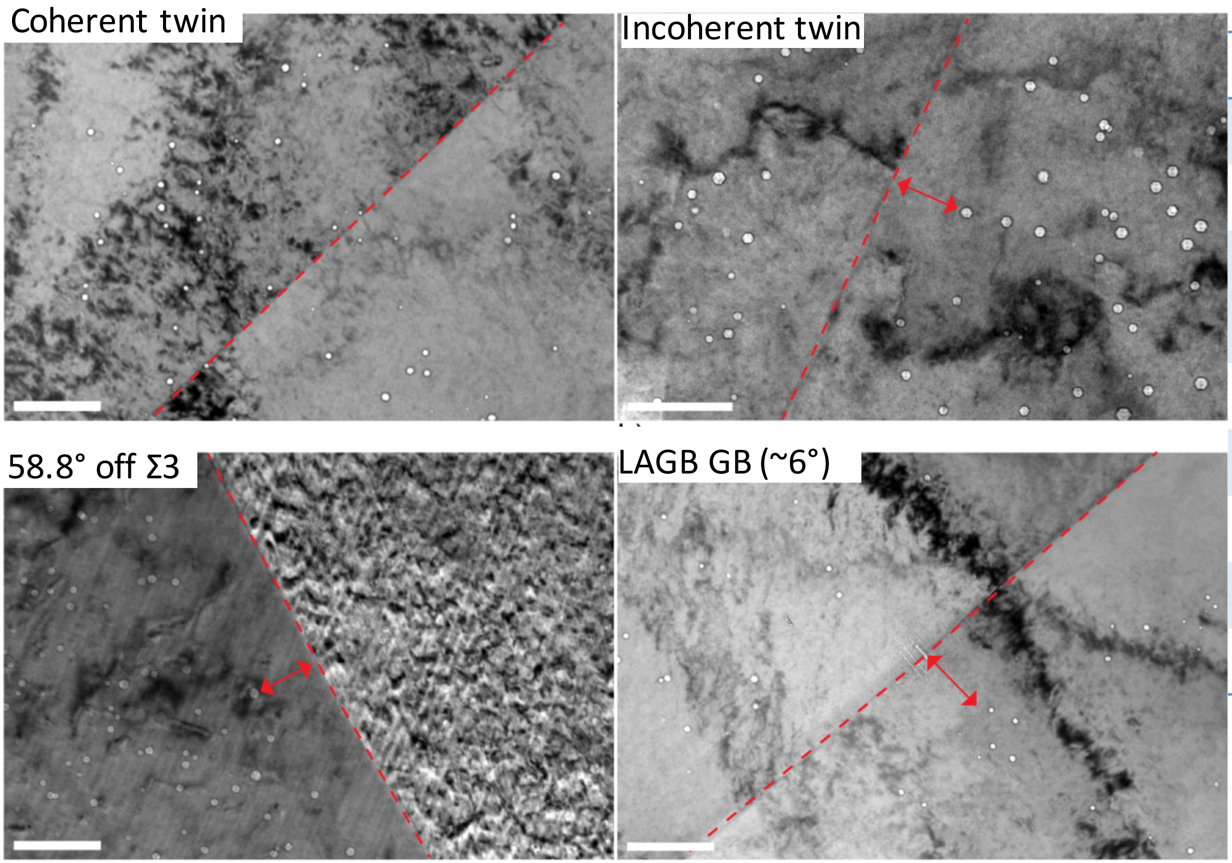
- Compared experimental RIS values to Wiedersich type rate theory model of RIS in Ni-Cr
- Modified to account differences in sink strength based on misorientation (and plane for Σ3 system)
- Bias is greater for the vacancy mechanism, which result in Cr depletion by RIS
- Comparison yields good agreement in high angle regime and for the coherent twin
- Low angle GBs RIS is underestimated compared to experiment



Barnard and Morgan, JNM 2014



GB Character Irradiation – Void Denuded Zones



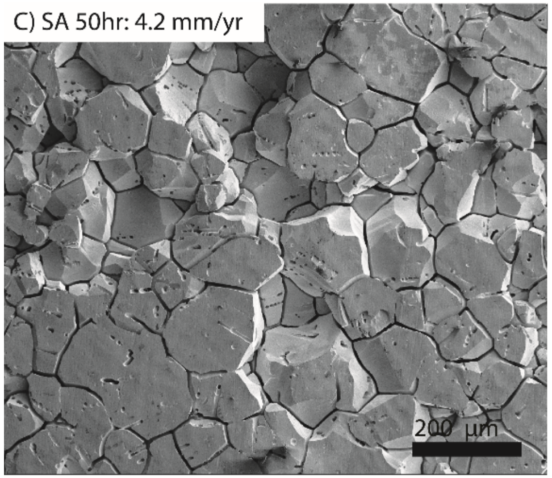
Scale bars = 200 nm

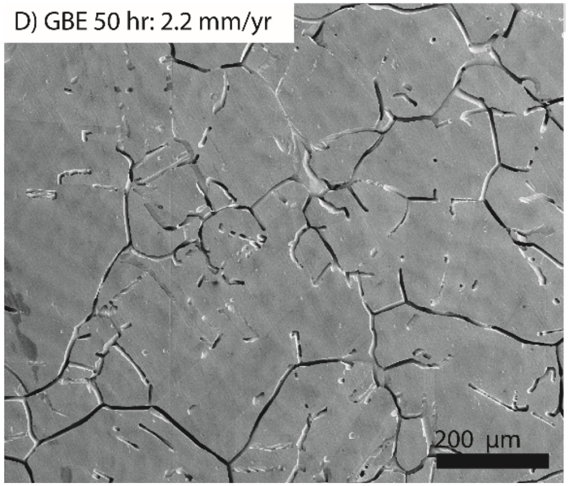
GB Character	VDZ Avg.
60° <111> {111} Σ3	0
60° <111> {112} Σ3	128
58.8° <14 17 12>, Σ3 Dev=8.2	115
59.0° <13 11 18>	155
56.6° <15 8 13>	145
47.1° <8 15 11>	137
14.2° <19 18 1>	135
6.1° <17 16 14>	132

- Minimal different in low verse high angle VDZ behavior based on misorientation angle
- Indicates misorientation (only 3 of 5 DOF) insufficient to determine GB sink efficiency
- Observed asymmetry in VDZ in most GBs

Project Discussion and Outcomes in 316L:

- Effective light rolling followed by high temperature annealing induces formation of GBE microstructures consistent with large twin related domains in 316L
- RIS in 316 clearly indicate GB sink efficiency variations between coherent twin and incoherent twin while minimal difference in random HAGBs.
- GBE provides opportunity to increase Σ3 coherent length fraction → improved corrosion resistance and minimized Cr depletion during RIS





Project Discussion and Outcomes in Binary Ni-Cr:

- No apparent sink efficiency difference between random high and low angle GBs
- Highly anisotropic sink efficiency in Σ3 GB plane for RIS and VDZs. Agreement here in model-experimental approach.
- Sink efficiency increases with deviation from twin plane
- Breakdown in model-experiment at low angle GB – need for better estimate of solute-defect interactions in low angle GBs: GB energy insufficient boundary term for estimating RIS

- **Future Direction**:

1. Broader GB characters including Σ11 {113} tilt verse asymmetric tilt; screw and edge components of low angle GBs for point defect accommodation.
2. Determination of GB plane normal for random GBs

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Questions?

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