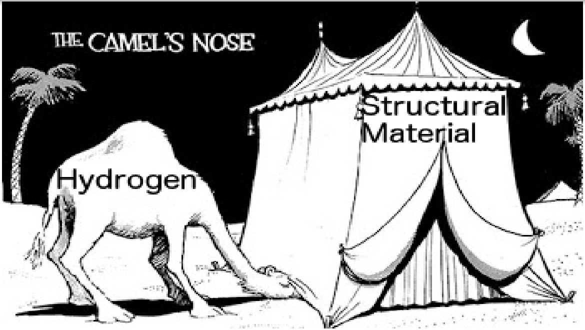
On the interaction of solu SAND2016-1111C
The Camel's Nose Analogy[1]



"If the camel once gets his nose in the tent, his body will soon follow."

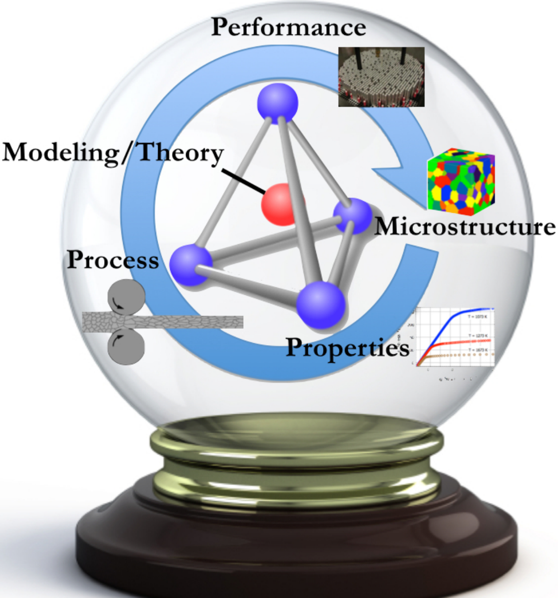
Sandia National Laboratories

[1] Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Collaborators

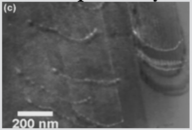
- Dr. Stéphane Berbenni: LEM3/CNRS, Metz, France.
- Dr. Chris O'Brien: Sandia Nat'l Labs, NM.
- Dr. Rick Karnesky: Sandia Nat'l Labs, CA.

Are material optimized designs mitigating environmentally-assisted aging in our future?



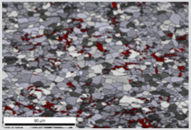
Hydrogen-assisted degradation limits structural performance

Hydrogen-enhanced local plasticity



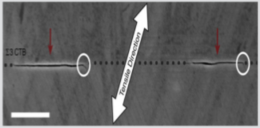
Ferreira, Acta Mater, 1998

Brittle hydride



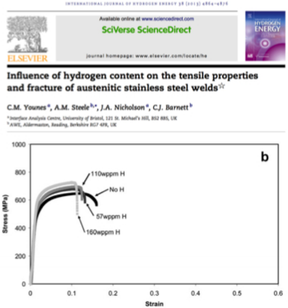
Kumar, J. Nucl. Mater, 2010

Hydrogen-assisted decohesion



Seita, Nature Comm, 2015

Loss of ductility



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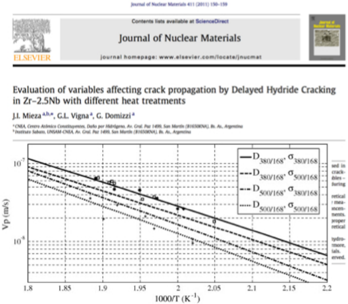
Influence of hydrogen content on the tensile properties and fracture of austenitic stainless steel welds☆

C.M. Younes[a], A.M. Steele[b,*], J.A. Nicholson[a], C.J. Barnett[b]

Hydride cracking



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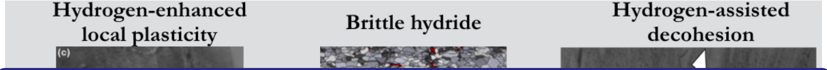
Evaluation of variables affecting crack propagation by Delayed Hydride Cracking in Zr–2.5Nb with different heat treatments

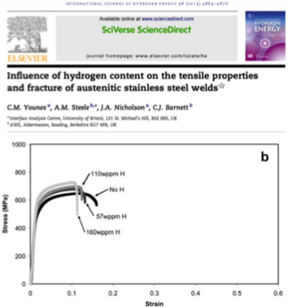
J.I. Mieza[a,b,*], G.L. Vigna[a], G. Domizzi[a]

Hydrogen-assisted degradation limits structural performance



Scientific questions to be addressed:

- Are there microstructures more susceptible to hydrogen-assisted intergranular fracture? If so,
  - What are the characteristics scales of importance?
  - What are the microstructural features (in the sense of GB engineering) impacting H segregation/embrittlement at GBs?



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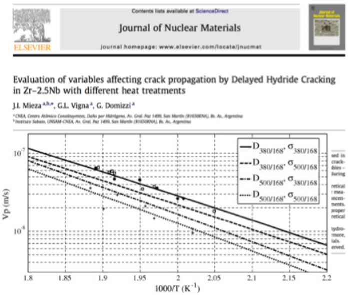

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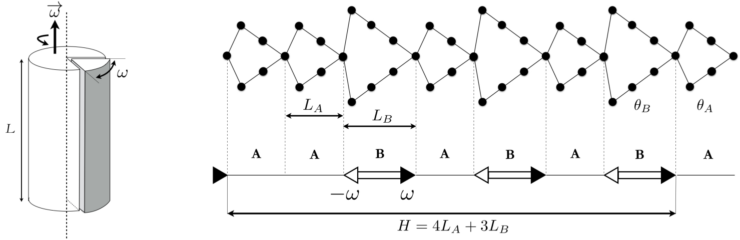
Evaluation of variables affecting crack propagation by Delayed Hydride Cracking in Zr–2.5Nb with different heat treatments

J.I. Mieza[a,b,*], G.L. Vigna[a], G. Domizzi[a]

Today's reflection and overview

1. **Where hydrogen matters...**
2. **Segregation susceptibility using continuum mechanics**
   - Grain boundary construct using disclination-based model
   - Fermi-Dirac statistics of site occupancy to model solute trapping at grain boundary
   - The importance of grain boundary character
   - Correlations with the Frank-Bilby formalism
3. **Perspective and summary**
   - Reality check

Construction of grain boundaries using the disclination structural unit model (DSUM): Nuts & bolts...



- Disclinations are linear rotational defects (logarithmic divergence of the long-range stress fields).
- Decomposing GB into a contiguous and alternating sequence of special (favored) m majority and n minority structural units.
- Boundary is represented in the form of a complex wall of disclinations combined into dipoles associated with the **minority structural units**.
- GB intrinsic stress field: $\sigma_{ij}^{\ddagger,mn} = \sum_{k=-\infty}^{\infty} \sigma_{ij}^{\bowtie}\left(x, y, \omega, L_n' + kH\right)$.

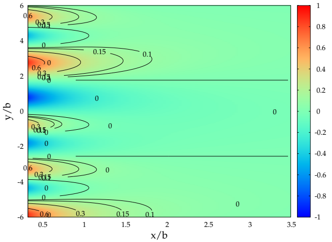
Symmetric tilt GBs about the [001] axis: structural character

θ [°]	GB plane	Σ	Structural decomposition of the period
0.00	(1 1 0)	1	|A|
16.26	(4 3 0)	25	|AAB.AAB|
20.02	(10 7 0)	149	|AABABAB.AABABAB|
22.62	(3 2 0)	13	|AB.AB|
25.06	(11 7 0)	85	|ABABABB|
28.07	(5 3 0)	17	|ABB|
36.87	(2 1 0)	5	|B.B|
43.60	(7 3 0)	29	|BBC|
46.40	(5 2 0)	29	|BC.BC|
53.13	(3 1 0)	5	|C|
58.11	(7 2 0)	53	|CCD.CCD|
61.93	(4 1 0)	17	|CD.CD|
64.94	(9 2 0)	85	|CDCDD.CDCDD|
67.38	(5 1 0)	13	|CDD|
73.74	(7 1 0)	25	|CDDDD|
90	(1 0 0)	1	|D|

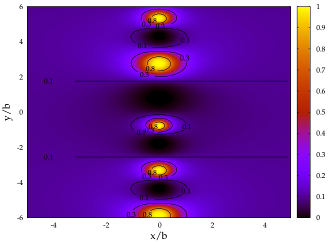
Fermi-Dirac statistics of site occupancy to model solute trapping at grain boundary

- Interstitial solutes = non-overlapping spherical misfitting inclusions with purely positive dilatational eigenstrain.
- Energetic contribution and the work done against pre-existing stresses upon the introduction of solutes.
- Solute field around GB:

$$\chi(\mathbf{x}) = \frac{1}{1 + \frac{1-\chi_0}{\chi_0} \exp\left(-\frac{1}{k_B T} \frac{1}{3} \sigma_{ii}^{\ddagger,mn}(\mathbf{x}) \Delta V \right)} .$$

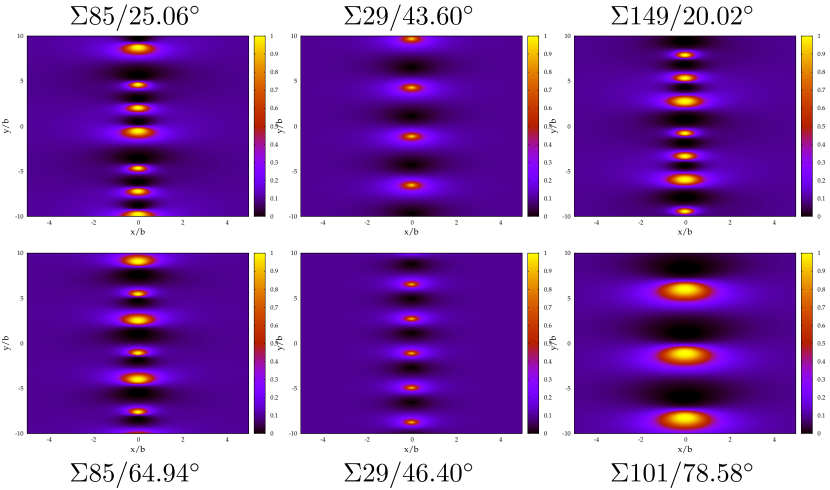


Hydrostatic stress field $\sigma_{ii}^{\ddagger,mn}$

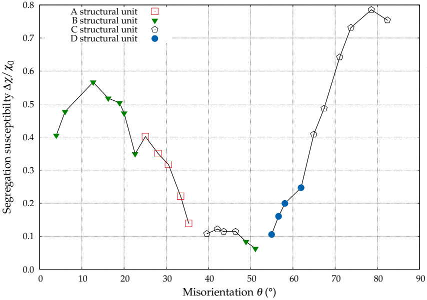


χ-field

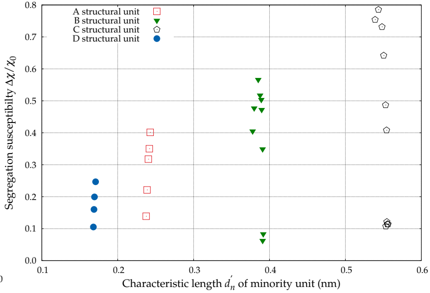
Solute fraction of occupied sites in the vicinity several grain boundaries



Segregation susceptibility variability is impacted by both the minority structural unit and the associated misorientation angle



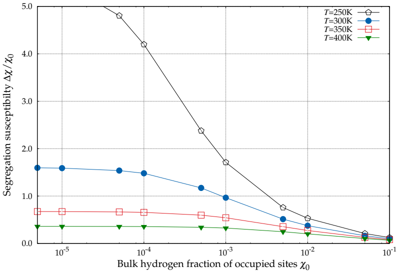
Segregation vs. misorientation.



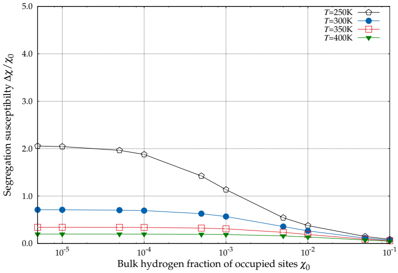
Segregation vs. characteristic length.

- Cusps corresponding to specific grain boundaries for which the structure changes from one minority structural unit to another.
- Three branches corresponding to pairs of structural units (A/B, B/C, C/D).

On the effect of temperature and prescribed bulk hydrogen fraction:



$\Sigma 17/28.07^\circ$ (B structural unit).



$\Sigma 17/61.93^\circ$ (D structural unit).

- Non-linear dependence on the prescribed bulk hydrogen content.
- Arrhenius-type dependence on the temperature.
- Solubility susceptibility less pronounced for GBs with misorientation θ in the range $36.87^\circ \leq \theta \leq 53.13^\circ$ (STGBs with only B and C structural units).

Frank-Bilby formalism

- Determine the intrinsic dislocation content of a general boundary.
- Burgers circuit construction, the net Burgers vector $\mathbf{B}_p$ of all interfacial dislocations crossing any vector **p** in the interface (i.e. closure failure in the perfect reference lattice)

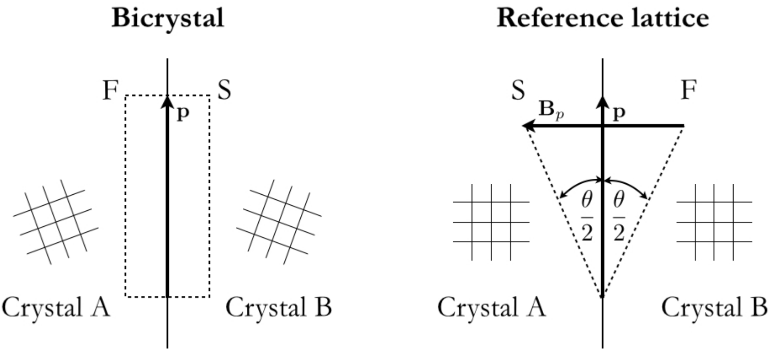
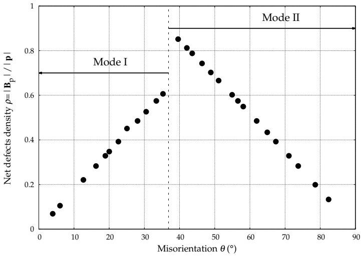
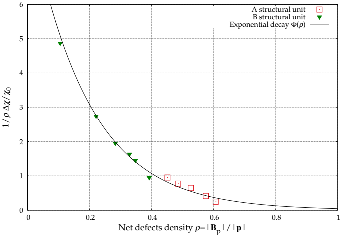


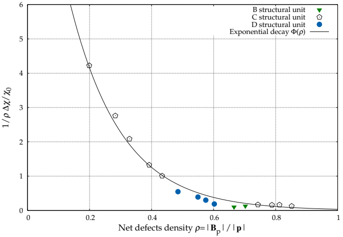
Illustration of the Frank-Bilby formalism for a symmetric tilt grain boundary.

Equivalence with the Franck-Bilby formalism





Mode “I”.



Mode “II”.

Segregation susceptibility within the Franck-Bilby formalism

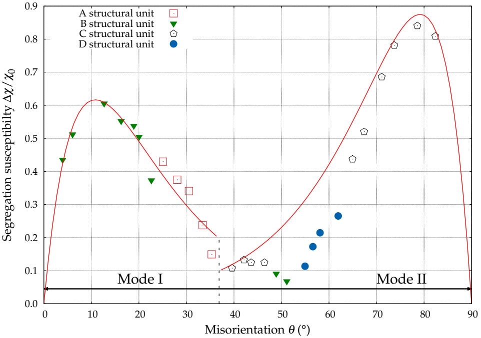
- Segregation susceptibility vs. net defect density:

$$\frac{\Delta\chi}{\chi_0}(\rho) = \rho\Phi_i(\rho), \text{ with } \rho = \frac{|\mathbf{B}_p|}{|\mathbf{p}|} = 2\sin\left(\frac{\theta}{2}\right)$$

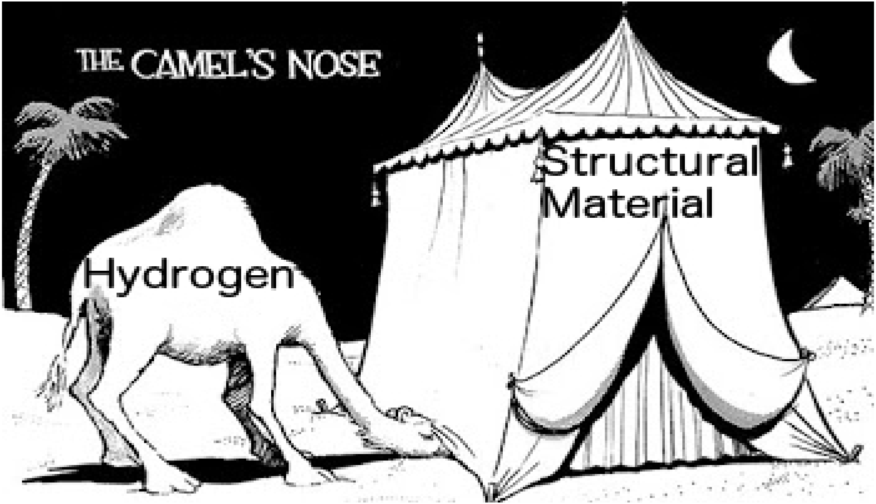
- Segregation susceptibility vs. misorientation:

$$\frac{\Delta\chi}{\chi_0}(\theta) = 2\sin\left(\frac{\theta}{2}\right)\Phi_I\left(2\sin\left(\frac{\theta}{2}\right)\right) \text{ for } \theta < 36.87^\circ$$

$$\frac{\Delta\chi}{\chi_0}(\theta) = 2\sin\left(\frac{90^\circ - \theta}{2}\right)\Phi_{II}\left(2\sin\left(\frac{90^\circ - \theta}{2}\right)\right) \text{ for } \theta > 36.87^\circ$$

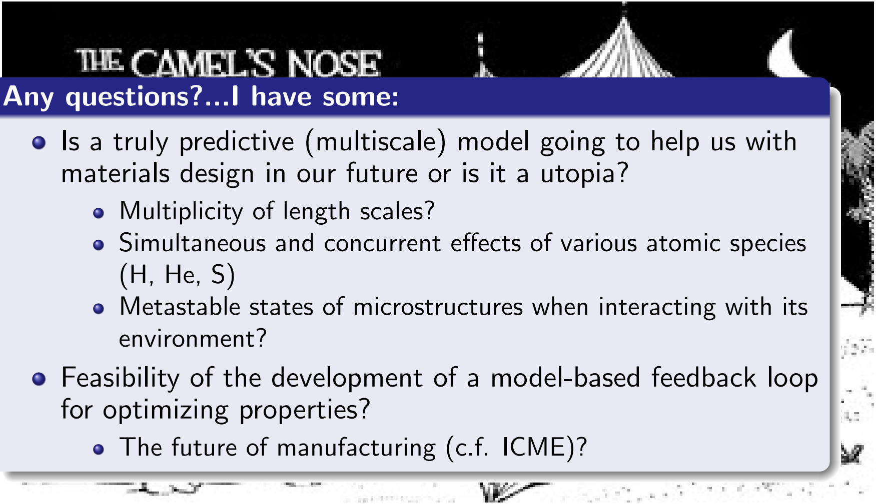


The camel's nose analogy...



"If the camel (H, He, S) once gets his nose in the tent (engineering materials), his body will soon follow (i.e. performance issues)."

The camel's nose analogy...



Any questions?...I have some:

- Is a truly predictive (multiscale) model going to help us with materials design in our future or is it a utopia?
  - Multiplicity of length scales?
  - Simultaneous and concurrent effects of various atomic species (H, He, S)
  - Metastable states of microstructures when interacting with its environment?
- Feasibility of the development of a model-based feedback loop for optimizing properties?
  - The future of manufacturing (c.f. ICME)?

"If the camel (H, He, S) once gets his nose in the tent (engineering materials), his body will soon follow (i.e. performance issues)."