Some Challenges to Multi-scale Modeling

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- First principles based microstructure modeling
  - *How close are we to directly modeling micro-structural modeling base on first principles parameter?*
    - *Vaithyanathan, C. Wolverton and L. Q. Chen, Physical Review Letters **88**, 125503 (2002)*
- Model problem for Fusion relevant Multi Scale Modeling
  - Oxide dispersion Strengthened (ODS) Alloys
  - *Why are nanoscale "clusters" stable at high temperature?*
    - *Janotti, Fu, Krcma, Miller, M&C ORNL*

Physical Review Letters **88**, 125503 (2002)

Multiscale Modeling of Precipitate Microstructure Evolution

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We demonstrate how three "state-of-the-art" techniques may be combined to build a bridge between atomistics and microstructure: (1) first-principles calculations, (2) a mixed-space cluster expansion approach, and (3) the diffuse-interface phase-field model. The first two methods are used to construct the driving forces for a phase-field microstructural model of θ'-Al_2Cu precipitates in Al: bulk, interfacial, and elastic energies. This multiscale approach allows one to isolate the physical effects responsible for precipitate microstructure evolution.

$$F_{\text{tot}} = F_{\text{bulk}} + F_{\text{inter}} + F_{\text{elast}} ,$$

$$F_{\text{bulk}} + F_{\text{inter}} = \int_V \left\{ f[c(\vec{r}), \eta_p(\vec{r})] + \frac{\alpha}{2} |\nabla c(\vec{r})|^2 + \frac{1}{2} \sum_{i,j}^{2} \beta_{ij}(p) \nabla_i \eta_p(\vec{r}) \nabla_j \eta_p(\vec{r}) \right\} dV$$

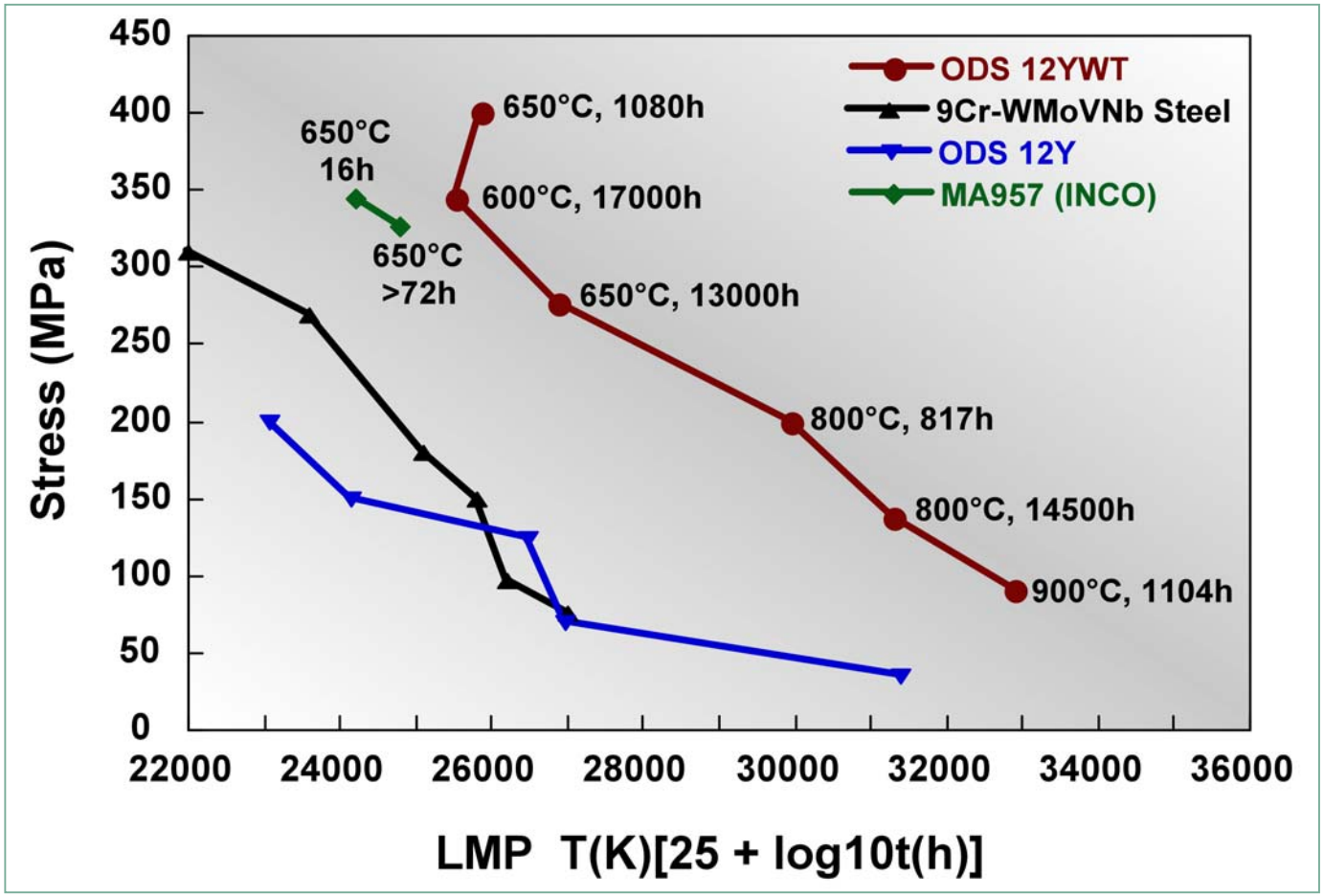
$$\frac{\partial c}{\partial t} = M \nabla^2 \left[\frac{\partial f}{\partial c} - \alpha \nabla^2 c \right],$$

$$\frac{\partial \eta_p}{\partial t} = -L(\phi_p) \left[\frac{\partial f}{\partial \eta_p} - \beta_{ii}(p) \nabla_i^2 \eta_p + \frac{\delta E_{el}}{\delta \eta_p} \right],$$

Oxide Dispersion Strengthen Alloys

Anderson Janotti, Chong Long Fu, Maja Krcma, Mike Miller,
Metals and Ceramics Division (ORNL)

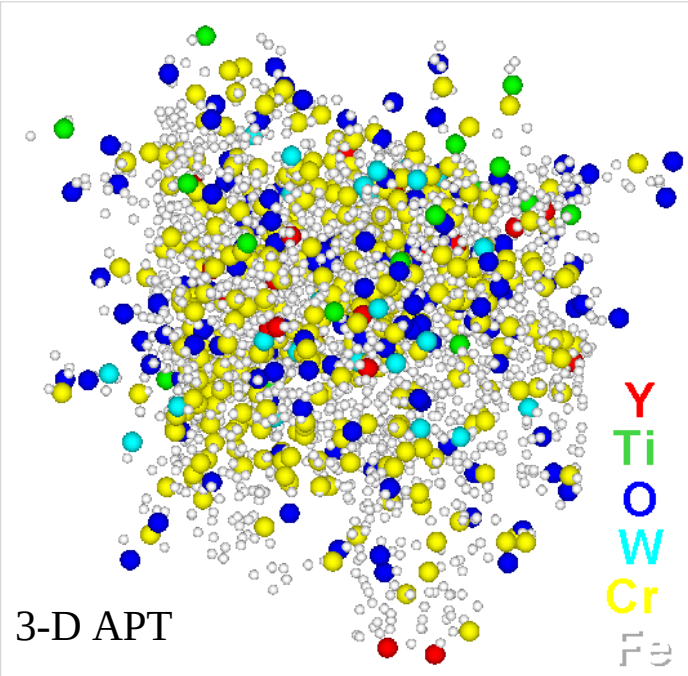
The 12YWT Ferritic Alloy Possesses Outstanding High Temperature Creep Strength

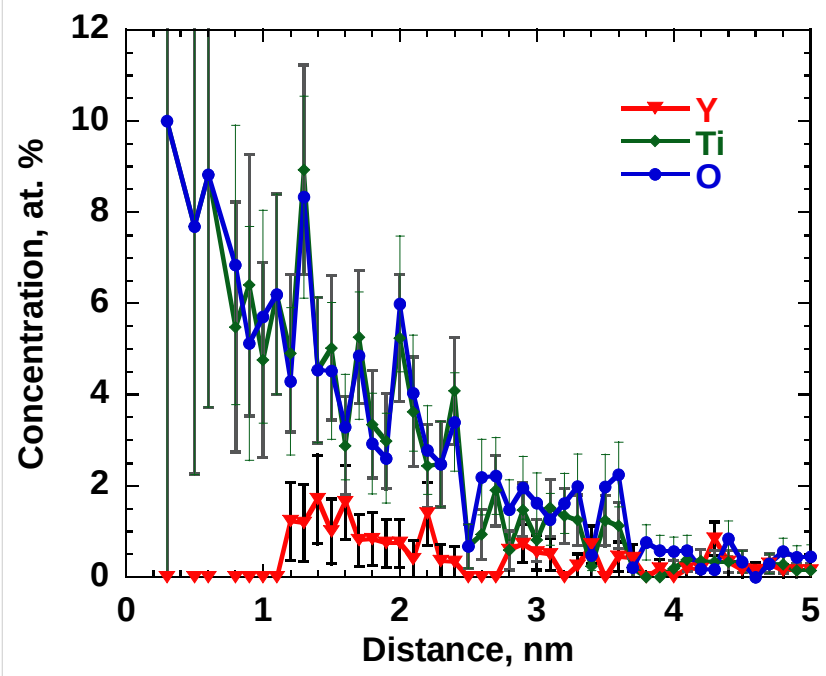


- *Creep rate is 6 orders of magnitude lower than conventional steels at 600-900ºC. (Larson-Miller Plot)*

Nanoclusters Are Enriched in Y, Ti, and O

- *Radial Concentration Profile (RCP) from the Center of Mass of a Particle*

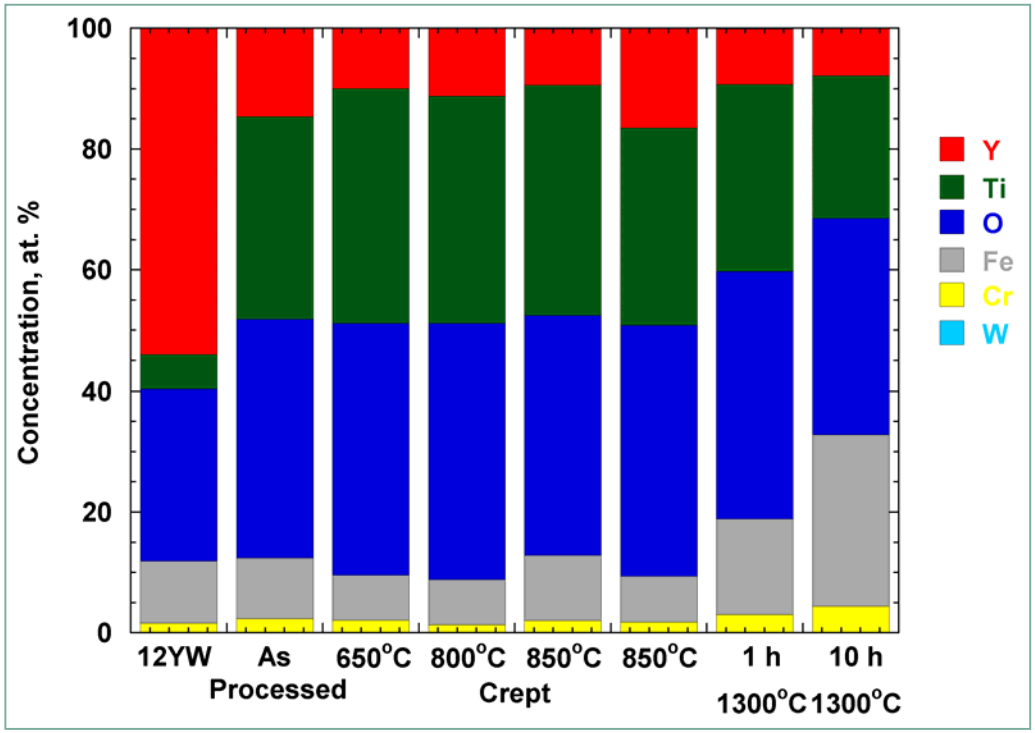




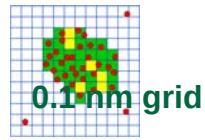
- No evidence of unique crystal structure in electron diffraction patterns
- RCP shows a diffuse interface structure

Nanoclusters Possess a High Degree of Thermal Stability

Compositions are the average of all nanoclusters analyzed in each condition



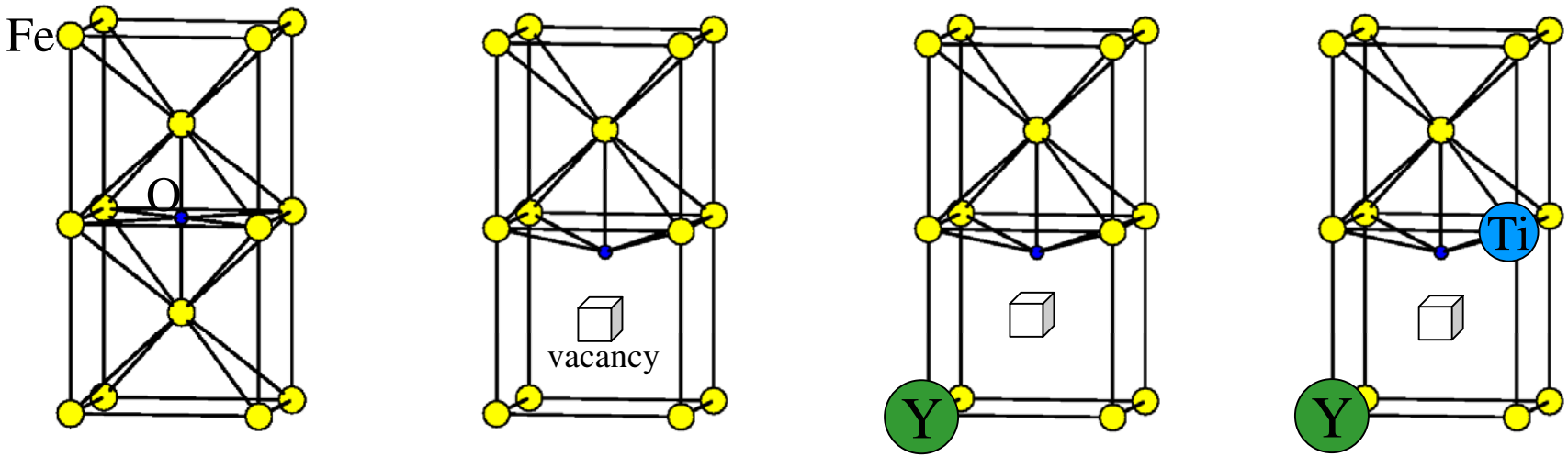
Maximum separation envelope method



- High-temperature exposures have little effect on the average composition of the nanoclusters
- The (Y+Ti):O ratio is ~1 in the 12YWT alloy
- The size of the ~4nm diameter nanoclusters does not change significantly during thermal ageing or creep
- ***The high degree of stability for the nanoclusters appears to defy the laws of thermodynamics***

Solubility of oxygen in Fe is strongly enhanced with Ti and Y additions

$$Fe/O \rightarrow Fe + FeO$$



$E_f = 1.5$ eV

Low oxygen solubility ~ 1-2 ppm at 900 C^o

1.9 eV (V-O_i pair)

Formation energy of V-O_i is 0.4 eV higher than that of O_i, despite high Fe vacancy formation energy ~ 2 eV

0.7 eV

Y significantly reduces the vacancy formation energy by 1.2 eV

~ 0 eV

Ti provides Ti-O chemical affinity

- **The reaction Fe:O/(Ti+Y) → Fe/(Ti+Y):O can be exothermic**
- **The presence of vacancy plays an indispensable role in O solubility enhancement (and in the cluster formation and stability)**