COMPUTATIONAL DESIGN AND PERFORMANCE PREDICTION OF CREEP-RESISTANT FERRITIC SUPERALLOYS

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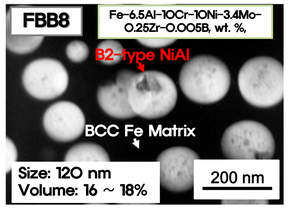
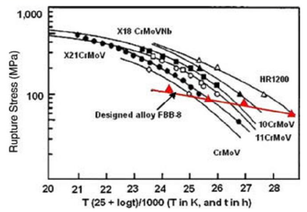
Introduction: NiAl-Strengthened Ferritic Alloys

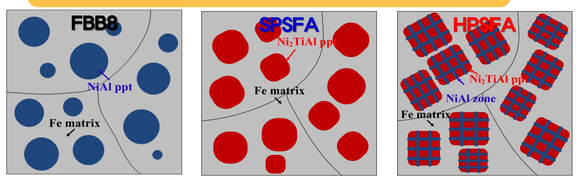


TEM dark field image of FBB8 along [100] zone axis using <100> superlattice reflection



A comparison of Larson-Miller parameter plots between FBB8 and other Fe-based materials candidates for steam turbine applications.

Objective



- Introduction of new types of precipitates, (single Ni_2TiAl precipitate-strengthened ferritic alloy [SPSFA], hierarchical Ni_2TiAl/NiAl precipitate-strengthened ferritic alloy [HPSFA].
- Understanding of the effect of precipitate structures on the creep behavior.

Schematic Illustration of Current Study

First-Principles Calculations

- Elastic Constant and Diffusion Coefficient
- Matrix/Precipitate Interface and Precipitate Morphology
- Effect of Elements on Coarsening

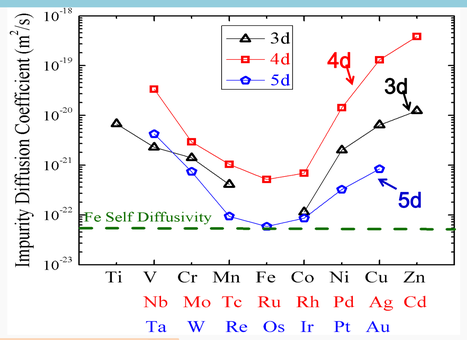
Experimental Validation

- Processing
  - Fabrication and Heat-Treatment
- Microstructural Characterization
  - Effects of Microstructures on Properties
- Creep and Mechanical Behavior
  - Deformation Mechanisms

Optimization of creep properties of novel ferritic superalloys with a hierarchical structure

First-Principles Calculations

Harmonic Transition-State Theory Assuming Vacancy Mechanism



$$D_A^B = D_{0_A}^B exp[-\frac{Q_A^B}{k_B T}]$$

ν^*: attempt frequency for the hop of a solute atom to a nearest-neighbor vacancy
ΔS_v^f: entropy of vacancy formation in bcc Fe
ΔH_v^f: sum of the vacancy formation energy in pure α-Fe
ΔH_m: migration energy for solute- vacancy exchange

Self Diffusion in a-Fe

$$D_{0_{Fe}}^{Fe} = a^2 f_{bcc} \exp\left[\frac{\Delta S_v^f}{k_B}\right] x \left[\frac{\prod_{i=1}^{3N-3} \nu_i^{vac}}{\prod_{i=1}^{3N-4} \nu_i^{sad}}\right]$$

$$Q_{Fe}^{Fe} = \Delta H_v^f + \Delta H_v^{mig,Fe}$$

ΔS_b: entropy of vacancy binding to a nearest-neighbor solute
ΔH_b: nearest-neighbor binding energy between a solute and vacancy

Impurity Diffusion

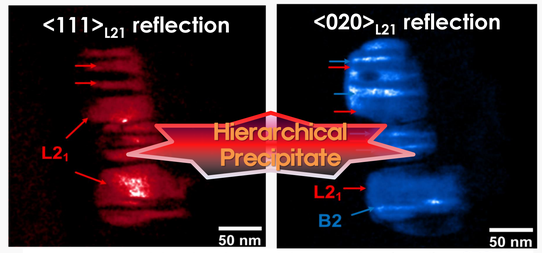
$$D_{0_{Fe}}^{I} = a^2 f_{Fe}^{I} exp\left[\frac{\Delta S_v^f + \Delta S_v^{bind}}{k_B}\right] x \left[\frac{\prod_{i=1}^{3N-3} \nu_i^{vac}}{\prod_{i=1}^{3N-4} \nu_i^{sad}}\right]$$

$$Q_{Fe}^{I} = \Delta H_v^f + \Delta H_v^{bind} + \Delta H_v^{mig,I}$$

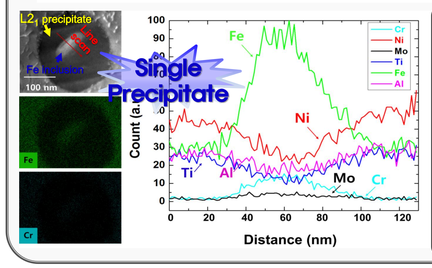
D_o: pre-exponential factor
Q_A: activation energy
a: lattice constant
f_2: correlation factor

Experimental Results

Fe-2Ti-6.5Al-10Cr-10Ni-3.4Mo-0.25Zr-0.005B (wt. %) → HPSFA

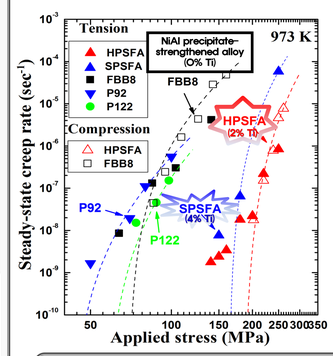


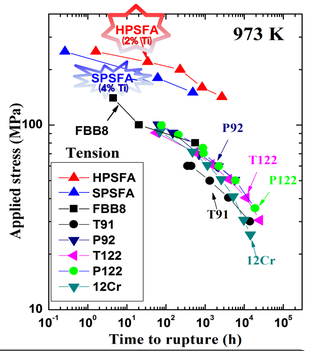
Fe-4Ti-6.5Al-10Cr-10Ni-3.4Mo-0.25Zr-0.005B (wt. %) → SPSFA



- **2%-Ti alloy** Hierarchical precipitate structure consisting of B2-NiAl and $L2_1$-Ni_2TiAl phases → **HPSFA**
- **4%-Ti alloy** Single-phase $L2_1$-Ni_2TiAl precipitate structure → **SPSFA**

Creep Properties



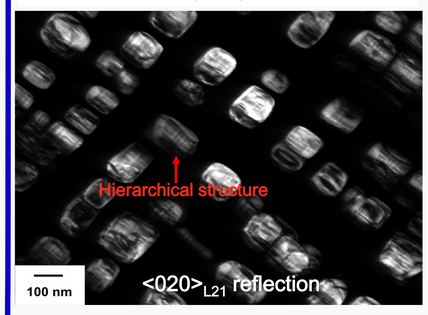


- HPSFA and SPSFA → Superior creep resistance to FBB8 and other ferritic steels
- HPSFA → Strain rates are more than four orders of magnitude lower than FBB8.
- HPSFA is much better creep resistant than SPSFA

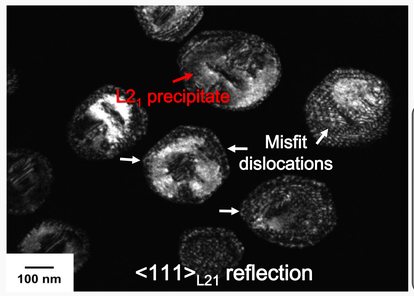
→ Indication of effective strengthening of Ni_2TiAl phase and hierarchical precipitate structures, as compared to that of the single NiAl precipitate.

Dark-Field Transmission-Electron Micrograph

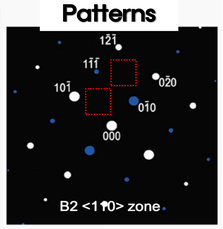
Fe-2Ti-6.5Al-10Cr-10Ni-3.4Mo-0.25Zr-0.005B (wt. %)

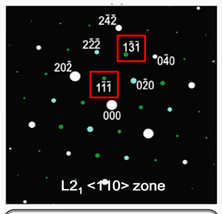


Fe-4Ti-6.5Al-10Cr-10Ni-3.4Mo-0.25Zr-0.005B (wt. %)



Simulated Patterns



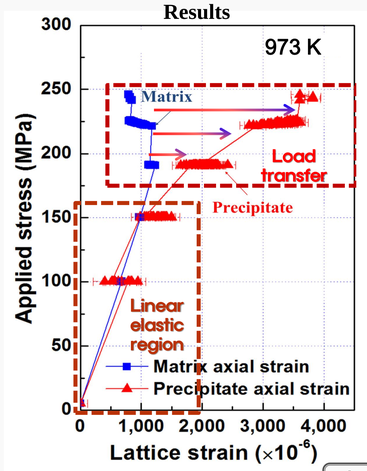


- **2%-Ti alloy** Cuboidal and coherent precipitates
- **4%-Ti alloy** Spherical and semi-coherent precipitates

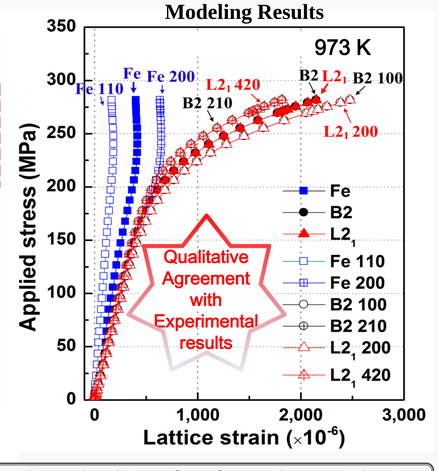
In-Situ Neutron-Diffraction Creep Results

Fe-6.5Al-10Cr-10Ni-3.4Mo-2.0Ti-0.25Zr-0.005B (wt. %), HPSFA

In-Situ Neutron Diffraction Experiment Results



Crystal-Plasticity Finite-Element-Modeling Results



(Lattice strain) $\varepsilon = \frac{a - a_0}{a_0}$

a = lattice parameter under loading
a_0 = lattice parameter without loading

- A clear load-transfer from the matrix to precipitate during loading and creep at 973 K.

→ Indication of insufficient diffusional flow at the matrix/precipitate interface.

Future Works

1. Effects of aging temperatures and time on the hierarchical-precipitate structure and creep behavior of the 2% Ti alloy (coarsening behavior and optimization of the creep properties)
2. Systematic study of hierarchical-precipitate-strengthened ferritic alloys by substituting Ti with Hf, Ta, and Zr (Introduction of the new hierarchical-precipitate structure and its effect on the creep mechanisms)
3. Systematic creep experiments at various temperatures and stresses on the new hierarchical-precipitate-strengthened ferritic alloys (study of creep behavior and mechanisms)
4. Calculations of single-crystal elastic constants (C_{ij}) for $L2_1$-Ni_2HfAl, $L2_1$-Ni_2TaAl, and $L2_1$-Ni_2ZrAl from first principles (morphology of precipitates and load-partitioning condition in creep studies)
5. Calculations of interfacial energies for BCC-Fe/$L2_1$-Ni_2HfAl (or $L2_1$-Ni_2TaAl, $L2_1$-Ni_2ZrAl from first principles (nucleation, coarsening resistance, and morphology of precipitates)
6. Dislocation-dynamic simulations to calculate the yield strength at room-temperature and creep-flow strength at high temperatures with various microstructures (controlling alloy microstructures to optimize the creep resistance)

Summary

1. Impurity-diffusion coefficients of 3d, 4d, and 5d in the BCC Fe matrix are calculated from first principles. It was found that the Impurity diffusion minimum for transition metal solutes is in middle of series (Ru and Os), with 5d < 3d < 4d.
2. TEM was conducted on 2% and 4% Ti alloys. It was found that the 2% Ti alloy contains a NiAl/Ni_2TiAl hierarchical precipitate, while the 4% Ti alloy consists of a single Ni_2TiAl precipitate.
3. These alloys are superior creep resistant at 973 K, as compared to the FBB8 and conventional ferritic steels. In particular, the creep rate of the 2% Ti alloy with the hierarchical precipitates is four orders of magnitude lower than FBB8.
4. From the in-situ neutron-diffraction experiments, a clear load transfer from the matrix to precipitate was observed during loading and creep deformation, which indicates the insignificant diffusional flow at the interface.
5. A crystal-plasticity finite-element model (CPFEM) shows reasonably good agreement with neutron-diffraction measurements.

Publications

1. Huang, S., Gao, Y., An, K., Zheng, L., Wu, W., Teng, Z. & Liaw, P. K. Acta Mater. 83, 137-148, (2015).
2. Liebscher, C. H., Radmilović, V. R., Dahmen, U., Vo, N. Q., Dunand, D. C., Asta, M. & Ghosh, G. Acta Mater. 92, 220-232, (2015).
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4. Teng, Z. K., Ghosh, G. Miller, M. K. Huang, S., Clausen, B., Brown, D. W., Liaw, P. K. Acta Mater. 60, 5362-5369, (2012).
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Acknowledgements

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