Computational Design of High Temperature Cast Aluminum For High-Efficiency Engines, PSED Cluster 2013-2014

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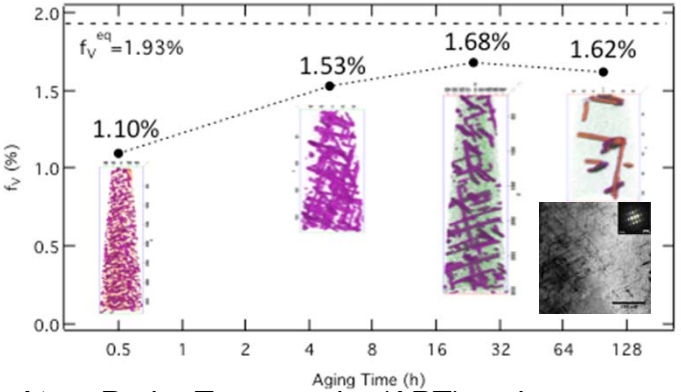
RESEARCH OBJECTIVE:

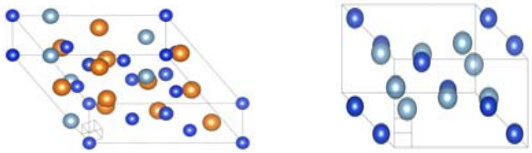
Implementation of Integrated Computational Materials Engineering (ICME) tools to design a high-temperature fatigue resistant aluminum alloy for use in lightweight vehicles. To design for both macro-scale properties and multi-scale material structures down to the atomic scale over large time domains requires the use of experimental data (APT, TEM), atomistic simulations (DFT), and precipitation kinetic modeling (PrecipiCalc). Integrating predictive modeling enables long time scale property projections for applications in high-temperature high-efficient engine operating environments.

EXPERIMENTAL RESULTS:

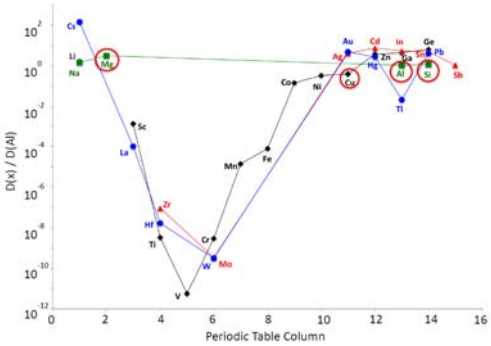


Atom Probe Tomography (APT) and Transmission Electron Microscopy (TEM) were performed on a two-phase FCC-Q alloy. Volume fraction, composition evolution, and particle size where measured as a function of aging time for use in model calibrations.

ATOMISTIC SIMULATIONS:

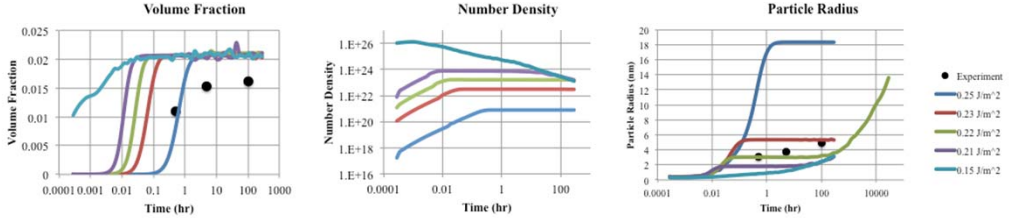


(a.) Q-phase and **(b.)** θ' -phase unit-cells used in DFT calculations



DFT calculations were performed to obtain solubilities for slow diffusing elements in both the Q and θ' strengthening phases for enhanced coarsening resistance.

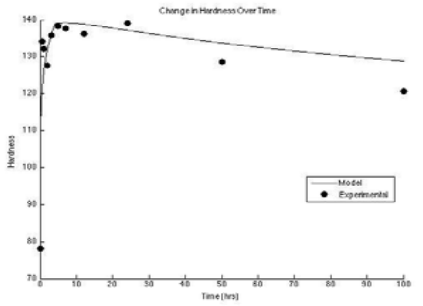
PRECIPITATION KINETICS:



PrecipiCalc simulations allow for the modeling of volume fraction, number density, and particle size as a function of aging temperature and aging time with varying interfacial energies and alloy compositions. Simulation and experimental results for the Q-phase exhibit similar trends for γ_Q=0.15 J m^{-2}.

PREDICTIVE MODELING:

A strength model was developed for the lath-shaped Q-phase. The model incorporated particle shear, Orowan-looping, and solid-solution hardening. Good agreement between experiment and the model has been demonstrated.



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