Fe-Cr Alloys for Advanced Nuclear Energy Applications

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The project objective is to exploit thermodynamic stabilization as an alternate means to control grain growth in model NFA's at elevated temperature, with the outcome that radiation damage tolerance can be improved by increase in the interfacial area/volume ratio, while also contributing to grain size strengthening mechanisms.

Thermodynamic Stabilization of Grain Size

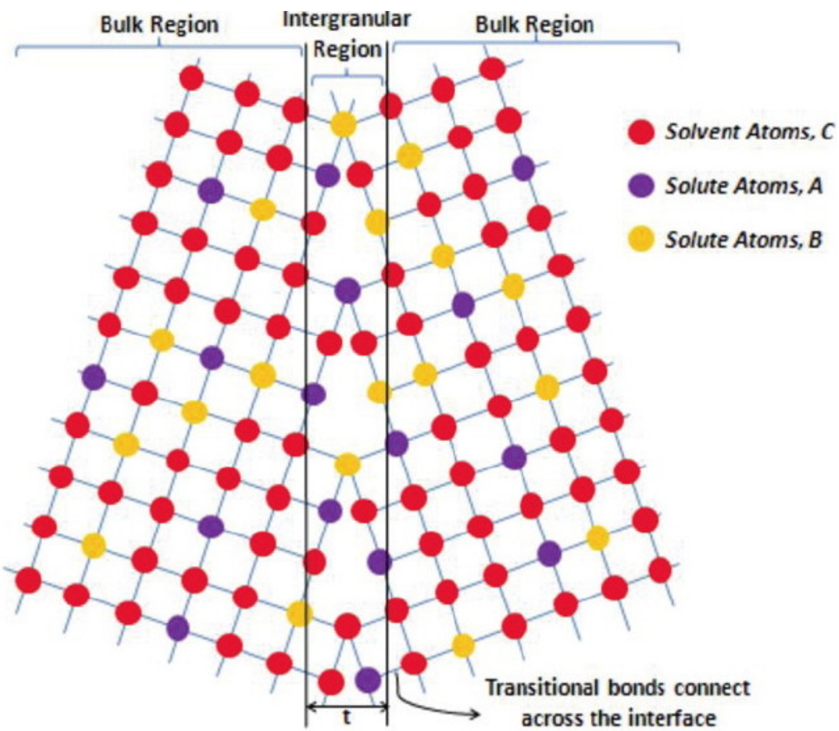
The concept is that *non-equilibrium* solutes introduced by mechanical alloying can segregate to grain boundaries, producing a minimum in the excess Gibbs free energy -> metastable equilibrium of the grain size at elevated temperatures.

A binary alloy (C + stabilization solute A) regular solution mixing model developed by Trelewicz and Schuh (TS)[1] properly minimizes the excess Gibbs free energy with respect to *both* interfacial solute concentration and grain boundary content – a critical step relative to previous models. The TS model includes bond interaction (chemical) enthalpy, but solute size misfit (elastic) enthalpy is ignored. In previous work, we extended the TS binary model to include elastic enthalpy, and also developed an effective computational scheme for numerical evaluation[2].

A ternary alloy (CB + stabilization solute A) introduces additional chemical and elastic interactions that can be very significant. We developed a ternary model as part of the NEET program[3], and use this for FeCrX alloy simulations.

1. J. R. Trelewicz and C. A. Schuh, Phys. Rev. B **79**, 094112 (2009)
2. M. Saber et al, J. Applied Phys. **113**, 063515 (2013)
3. M. Saber et al, J. Applied Phys., in review (2013)

Ternary model



Fe Cr A = C B A (at %)

Model Input data:

Elastic enthalpy $\Delta E < 0$

ΔE_{AC}

ΔE_{BC}

Chemical enthalpy $\Delta H = \omega z/4$

ΔH_{AC}

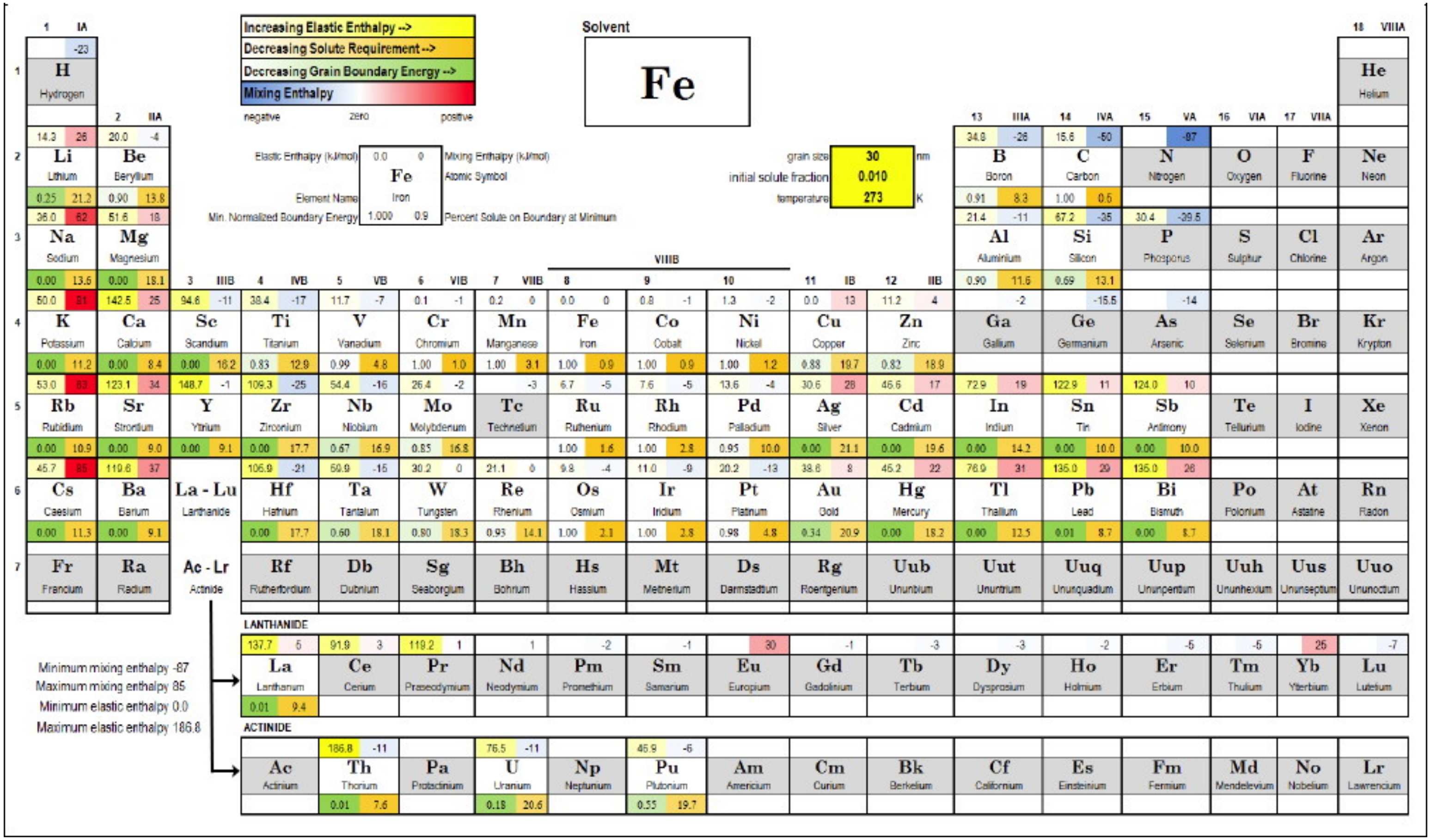
ΔH_{BC}

ΔH_{AB}

$\Delta H > 0$ -> phase separation

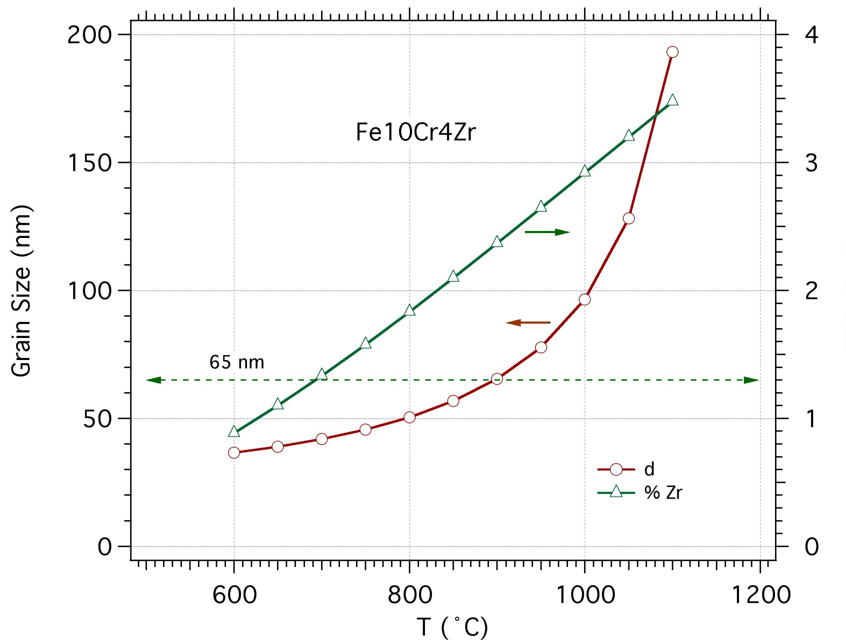
$\Delta H < 0$ -> phase formation

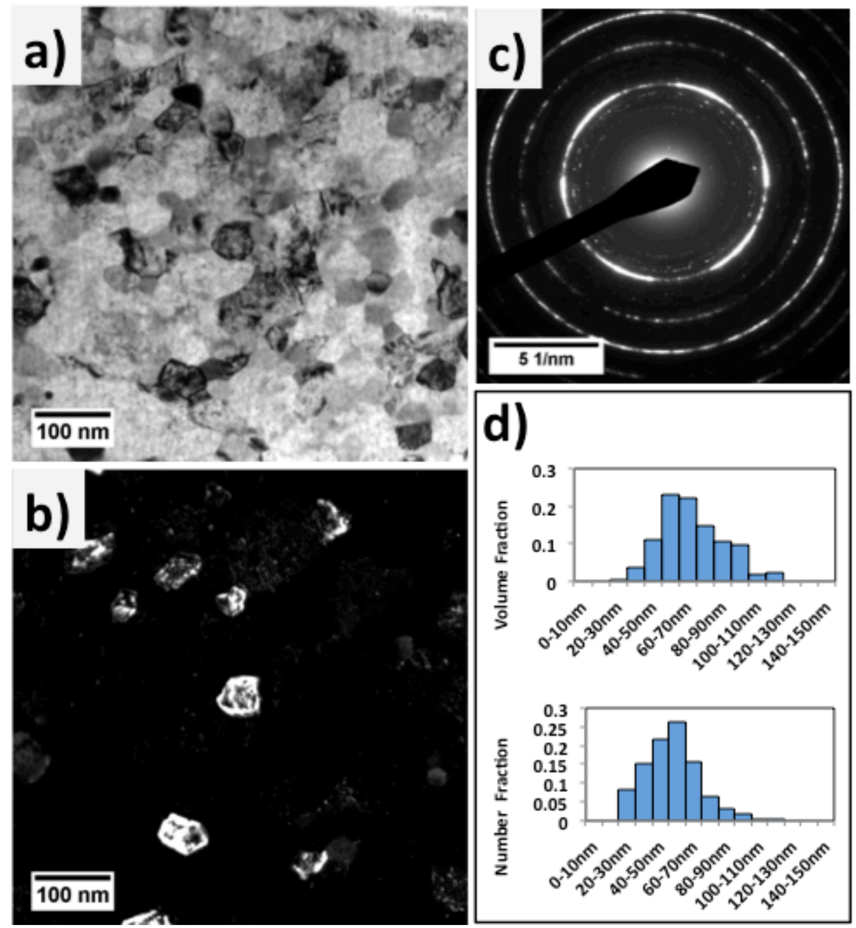
Input data compilation[1]



1. M. Atwater and K. Darling, ARL-TR-6007, May 2012

Fe10Cr4Zr simulation and experimental result for 900˚C

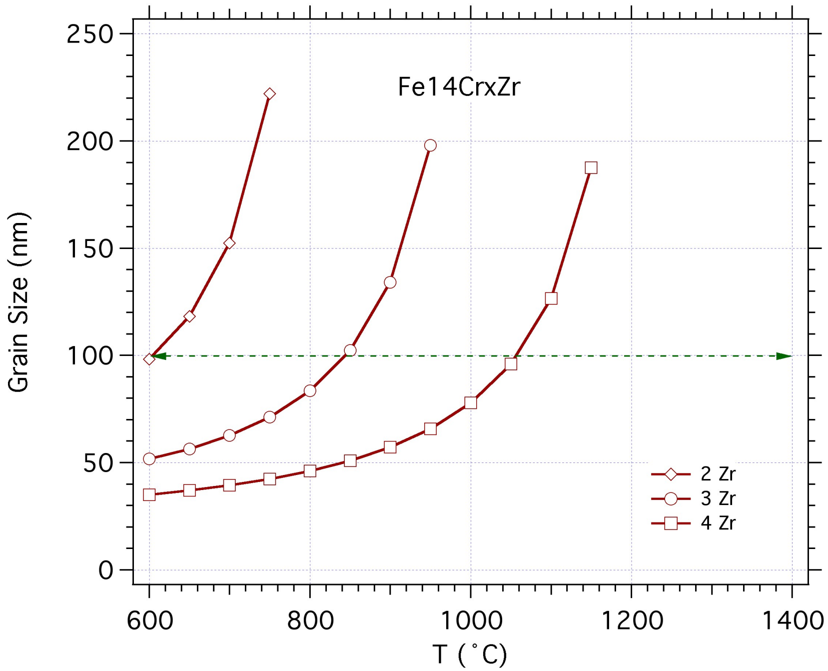


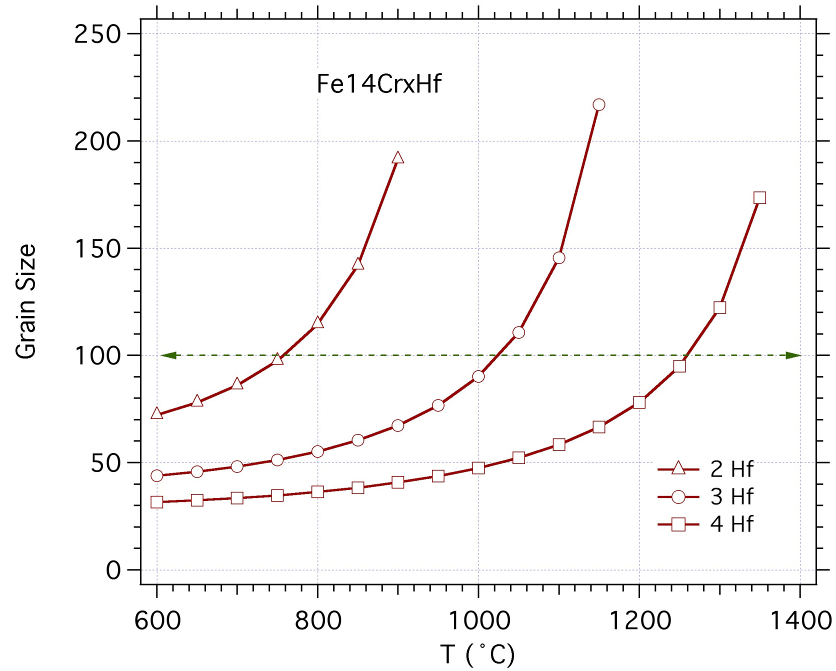


The simulation grain size at 900˚C = 65 nm and the solubility limit in the bulk is 2.3 %Zr. The SAD pattern indicates the presence of fine nanoscale intermetallic precipitates.

Volume average grain size = 58 nm

Simulations for Fe14CrxZr vs. Fe14CrxHf

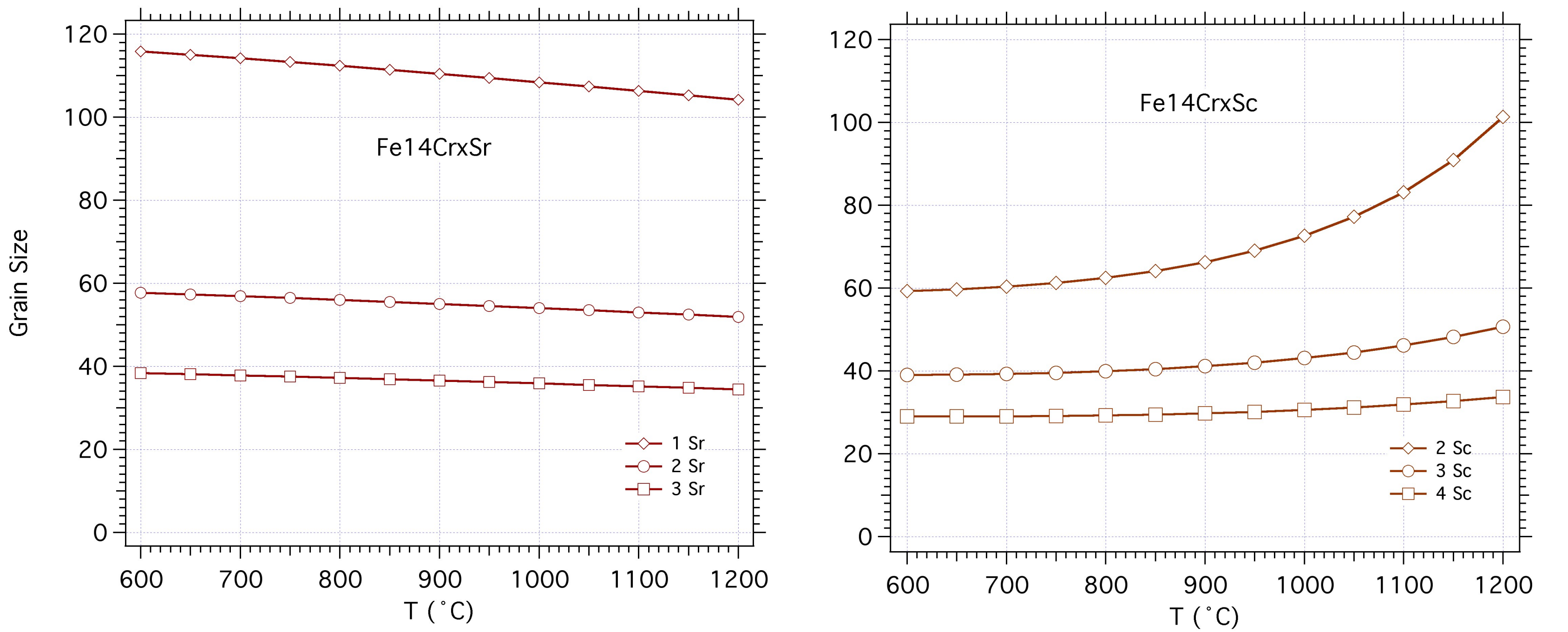




Hf is stronger than Zr for retaining nanoscale grain size at higher temperatures. Choosing a stabilizer solute has several aspects in addition to the grain size range. The melting points must be high and the expected resistance to grain-boundary embrittlement should be at least neutral[1]. Both Zr and Hf are favorable.

1. M. P. Seah, Proc. Royal Soc, London, A349 no. 1659, 535 (1976)

Simulations for Fe14CrxSr and Fe14CrxSc



Sr and Sc are very strong stabilizers up to high temperatures. The melting points are high and the bulk solubility is low, essentially zero for Fe14CrxSr. Grain boundary embittlement could be a concern[1]. Preliminary experiments will be done to evaluate these as stabilizers for Fe14Cr.

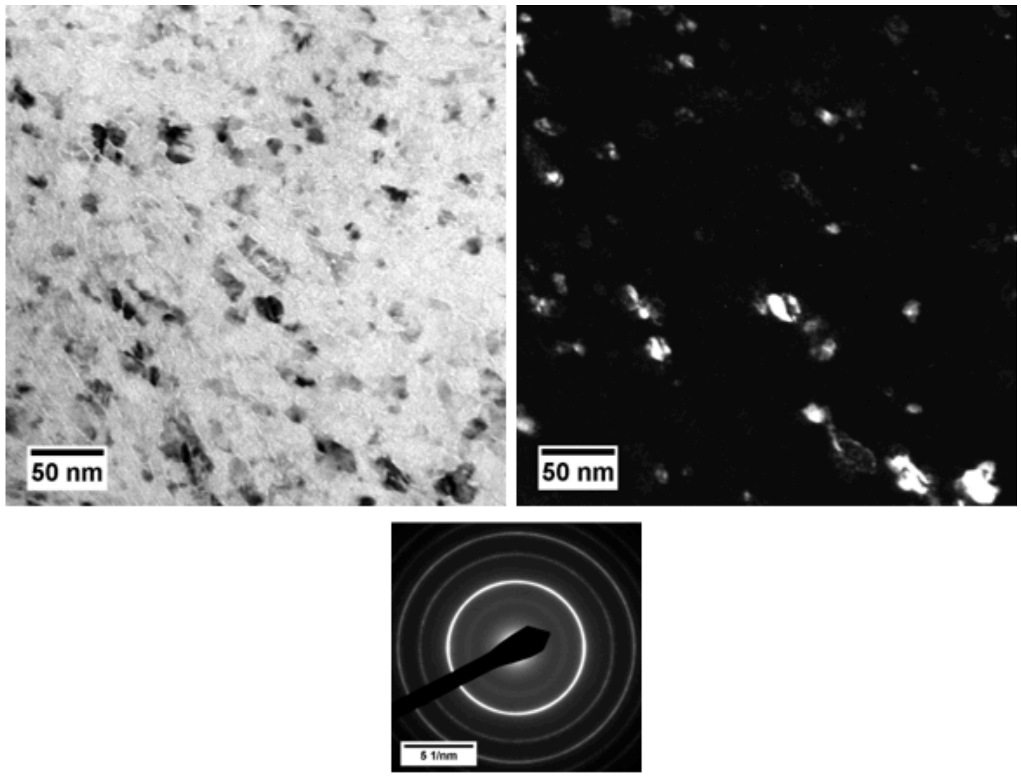
1. M. P. Seah, Proc. Royal Soc., London, A349 no.1659, 535 (1976)

Characterization of a base ODS NFA alloy $Fe\text{-}14Cr\text{-}0.4Ti\text{-}xY_2O_3$ (wt %)

All processing is done using SPEX milling

The target is x = 0.25. Values of x = 10 and 1 were used initially to investigate the Y_2O_3 distribution for nano and micron scale starting powders.

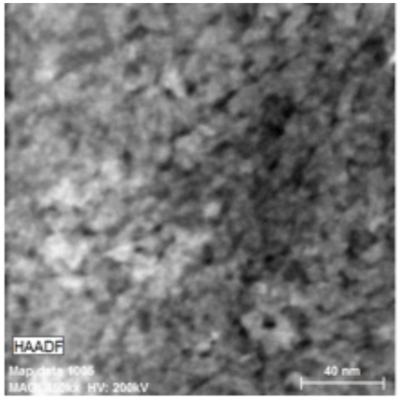
TEM for as milled Fe-14Cr-0.4Ti-10Y_2O_3

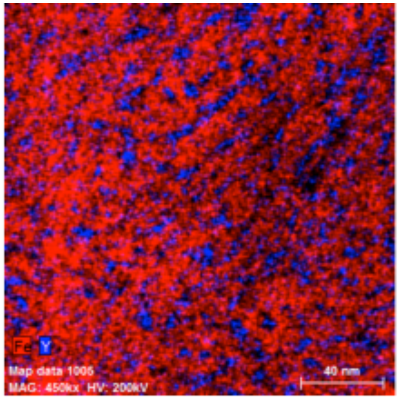


Results are independent of initial Y_2O_3 powder size. Grain size = 20 nm

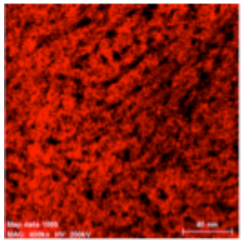
STEM for as milled Fe-14Cr-0.4Ti-10Y_2O_3

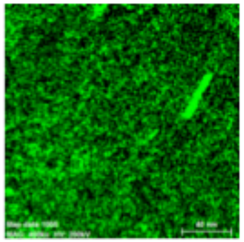
HAADF

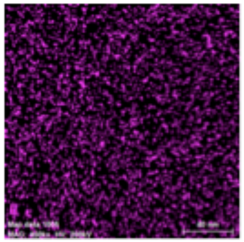


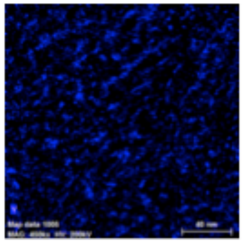


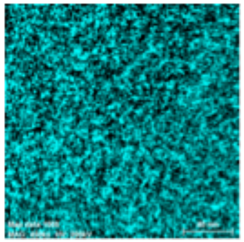
Fe-Y





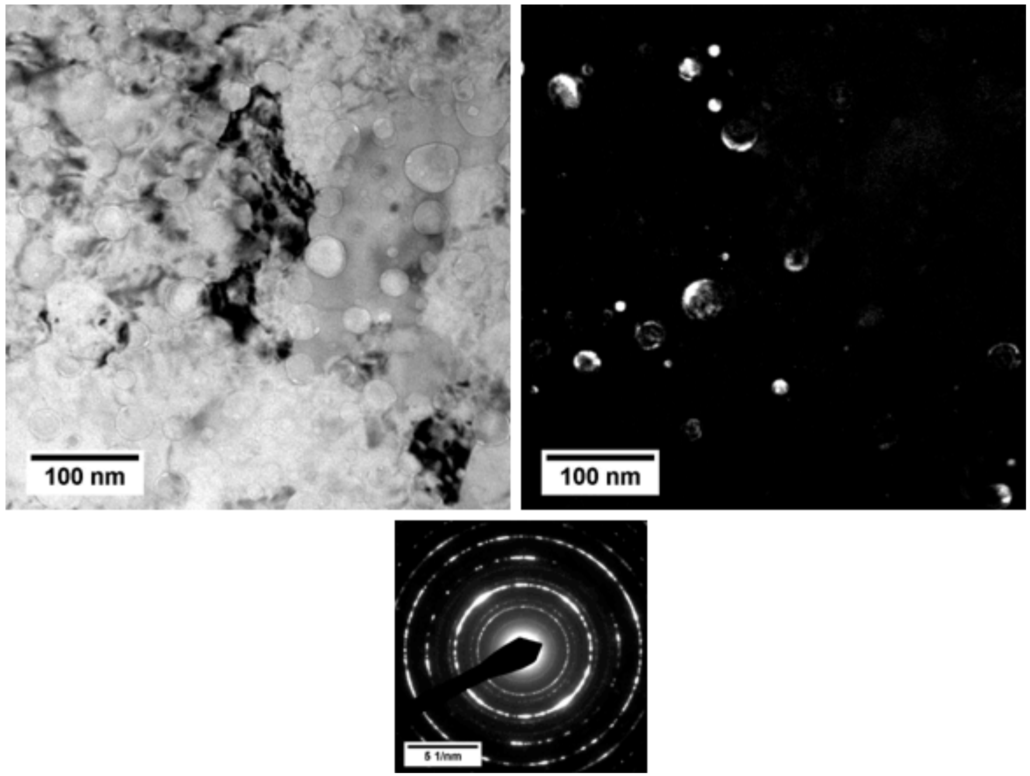






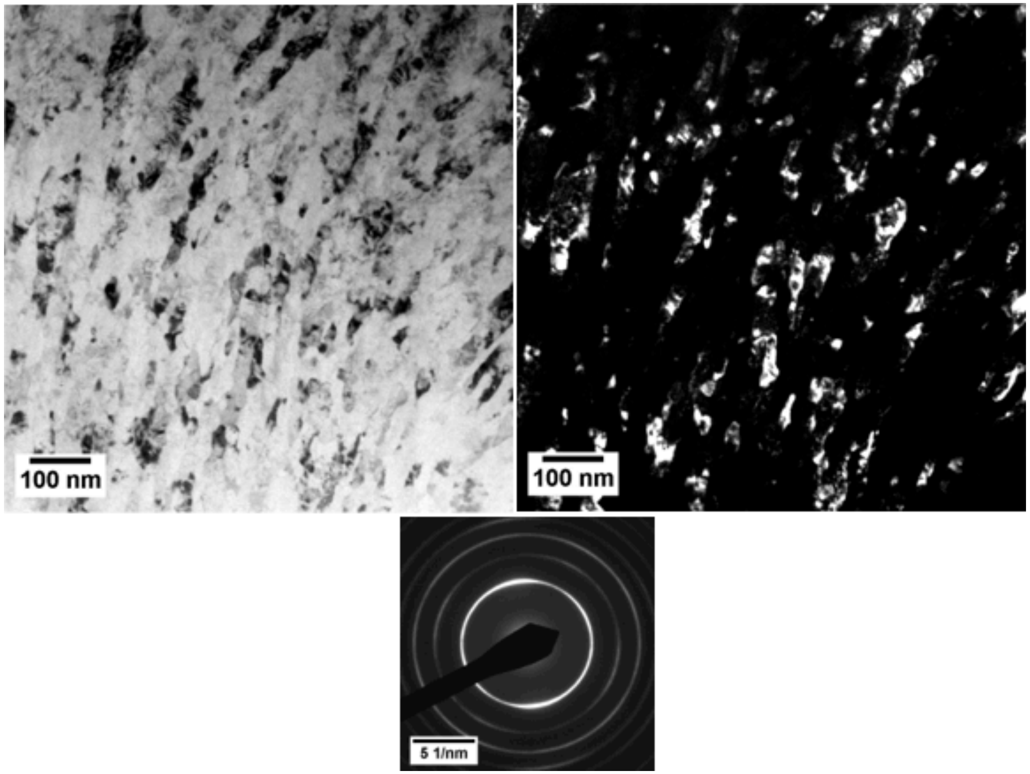
Fe Cr Ti Y O

TEM for $Fe\text{-}14Cr\text{-}0.4Ti\text{-}10Y_2O_3$ annealed at 1100C/1 hour



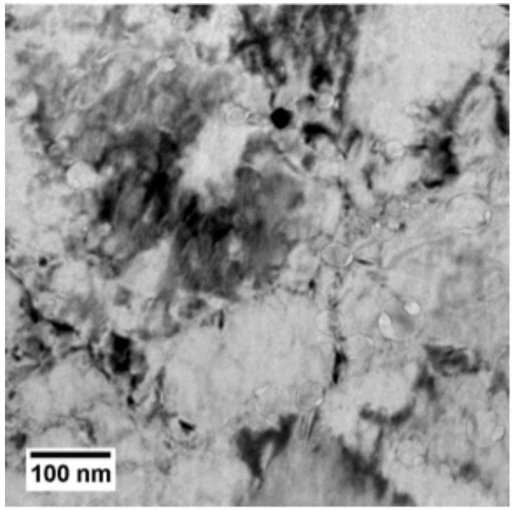
SAD (right image) isolates intermetallic precipitates

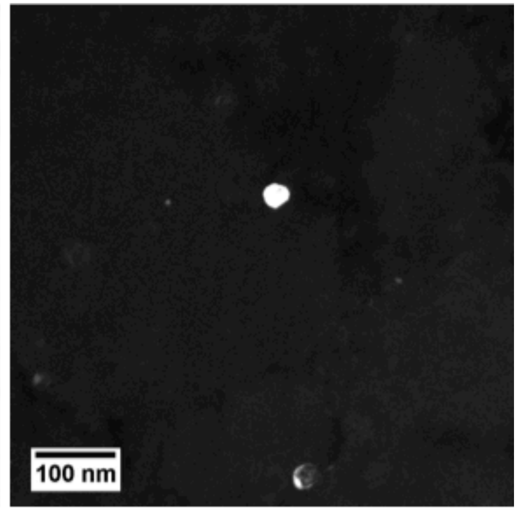
TEM for as milled Fe-14Cr-0.4Ti-1Y_2O_3

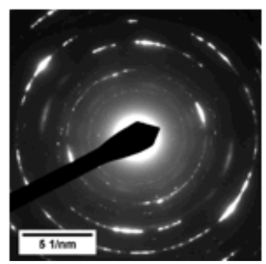


Results are independent of initial Y_2O_3 powder size. Grain size = 30 nm

TEM for Fe-14Cr-0.4Ti-1Y_2O_3 annealed at 1100C/1 hour

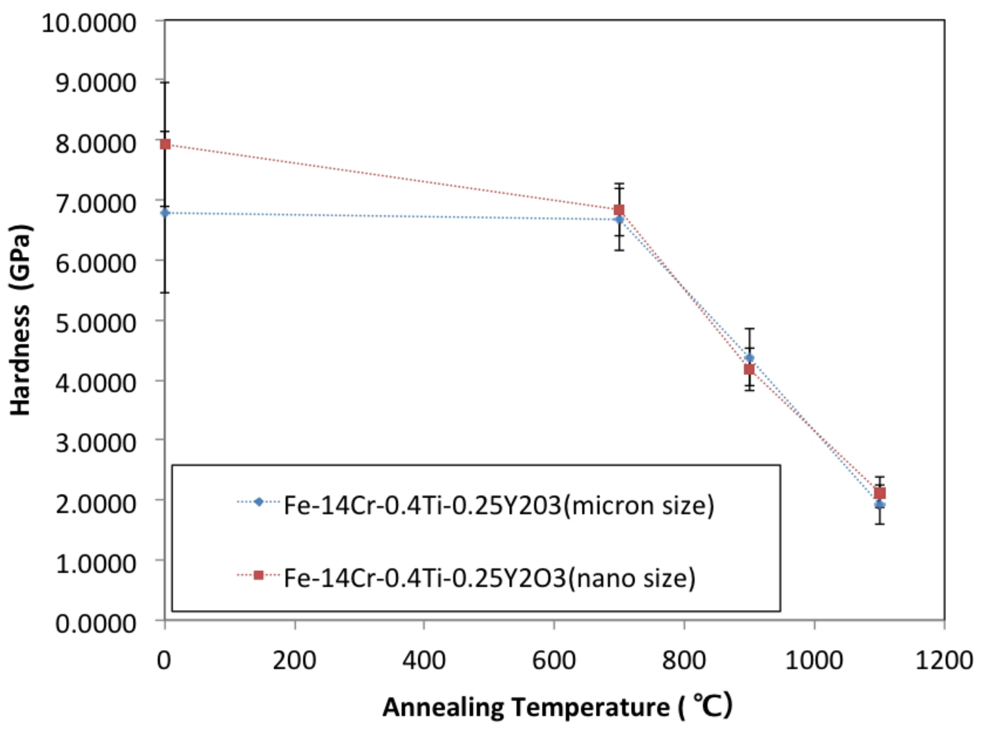






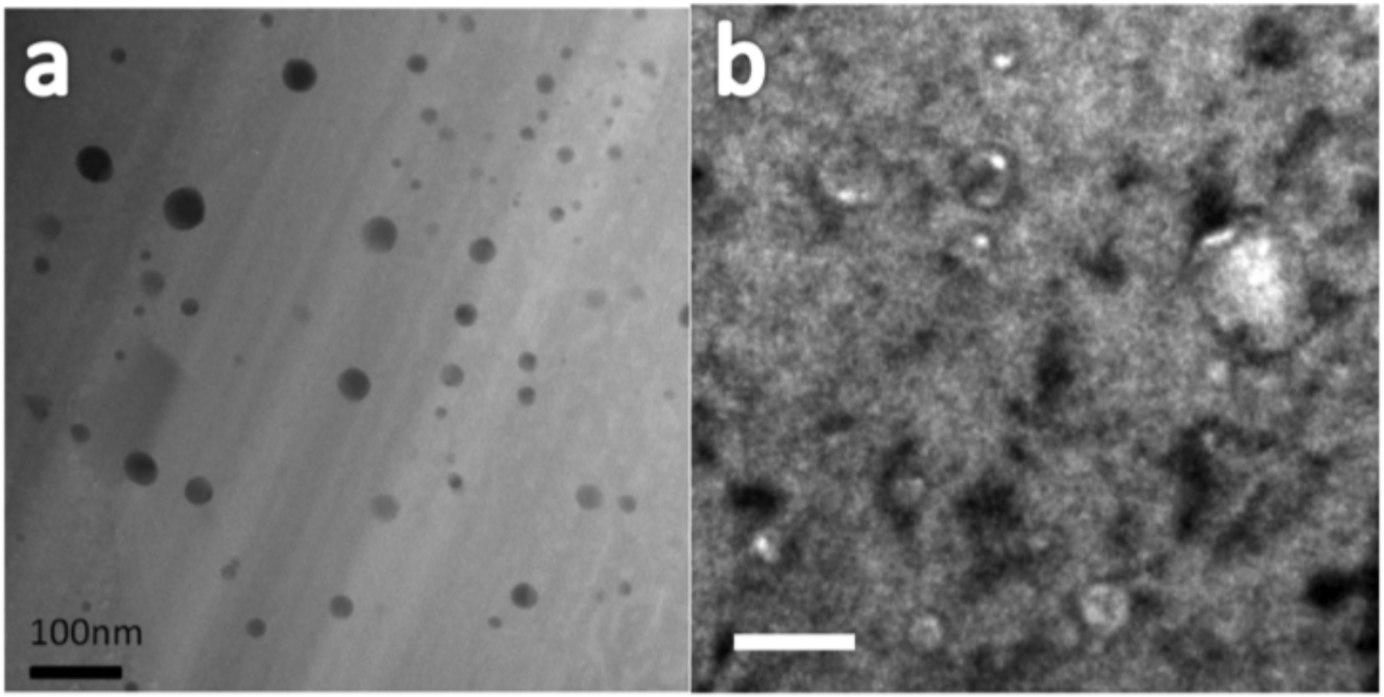
SAD (right image) isolates intermetallic precipitates

Microhardness vs. annealing temperature (1 hr) for Fe-14Cr-0.4Ti-0.25Y_2O_3



Hardness is measured on un-compacted powder particles

Microstructure of the Fe-14Cr-0.4Ti-0.25Y_2O_3 after 1100C annealing for one hour.
(a) High-angle annular dark-field (HAADF) image in STEM
(b) Bright-field image in TEM



Grain size > 100 nm

Elemental mapping of a typical oxide intermetallic precipitate (in the previous figure microstructure) by energy dispersive spectroscopy (EDS)

(a) HAADF image, (b)-(f) the major elements within the oxide are Fe, Cr, Y, Ti and O, respectively (40 nm scale bars).