Y-Ti-O nanocluster formation in Fe: A combined study using Density Functional Theory and Lattice Kinetic Monte Carlo simulations

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Introduction

- The strength of Nanostructured Ferritic Alloys depends on the distribution of Y-Ti-O nanoclusters in the matrix.
- These nanoclusters are formed during the high temperature consolidation of the ball milled (powdered) alloy.
- Understanding the initial phase of formation of these nanoclusters is crucial to predict their overall behavior.
- We have used first principles methods along with Lattice Kinetic Monte Carlo technique to study the kinetics of nanocluster formation in BCC Iron.

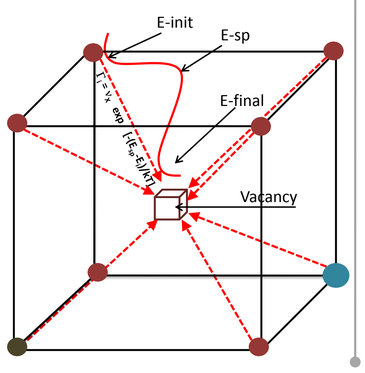
The LKMC Model

Two sublattices: 1st sublattice: regular bcc sites with Fe, Y, Ti, vacancy (□)
2nd sublattice: octahedral interstitial sites with Oxygen

One Monte Carlo sweep: all the Vacancy and O allowed to jump once

A rigid bond model for total energy with interactions up to second neighbor (fitted to first principle calculation)

$$E = \sum_{k} \sum_{i,j} \varepsilon_{ij}(k) n_{ij}(k)$$



The bond energies are calculated from Density Functional Theory using VASP code with PAW (PBE) psuedo potential with 128 atom supercell.

The migration barriers for the solute atoms in bcc iron were calculated using the Nudged Elastic Band (NEB) method

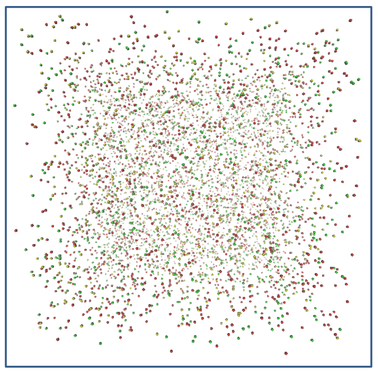
Migration Energy Barriers

	Migration energy E_m (eV)
Fe-□	0.65
Y-□	0.10
Ti-□	0.40
O	0.55

Pairwise bond energy parameters

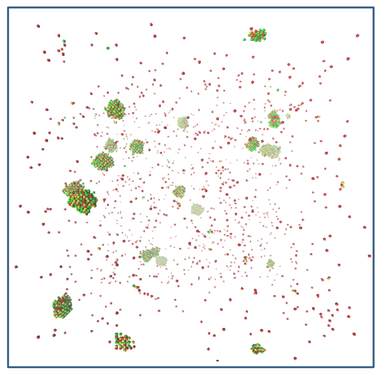
Pairwise bonds	First neighbour (eV)	Second neighbour (eV)
Fe-Y	0.25	0.00
Fe-Ti	-0.10	0.00
Fe-O	0.35	0.17
Fe-□	0.25	0.00
Y-Y	0.19	0.01
Y-Ti	0.15	0.01
Y-O	0.45	-1.05
Y-□	-1.40	-0.25
Ti-Ti	0.23	0.13
Ti-O	-0.25	-0.55
Ti-□	-0.25	0.16
□-□	0.15	-0.21
□-O	-1.55	-0.75
O-O	0.60	0.40

Formation of Y-Ti-O clusters

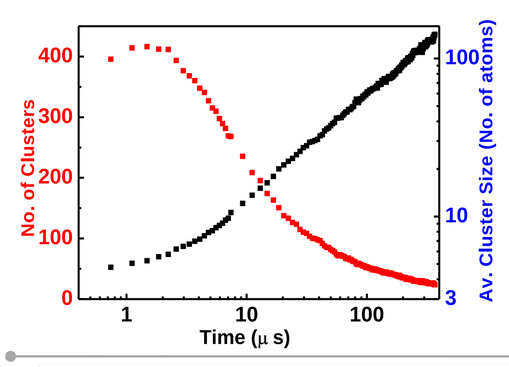


88 88 88 unit cells (1.3 million sites) Y: 0.12%, O: 0.2%, Vac: 1000 ppm Temp. 1150 K

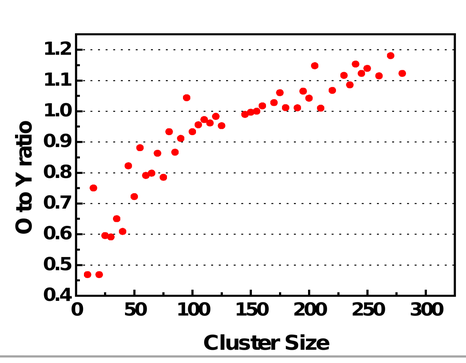
Randomly distributed Y, Ti, O and vacancy in Fe, evolved by vacancy jumps and interstitial O jumps, leading to the formation of clusters



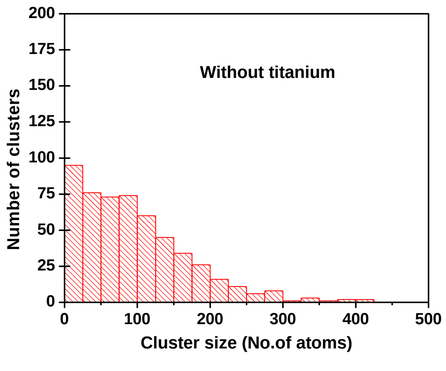
Evolution of clusters with time

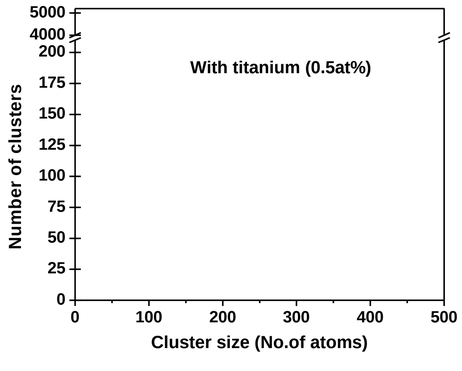


O to Y ratio in the clusters

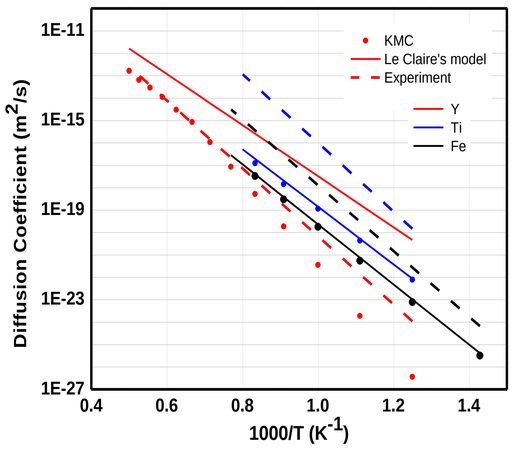


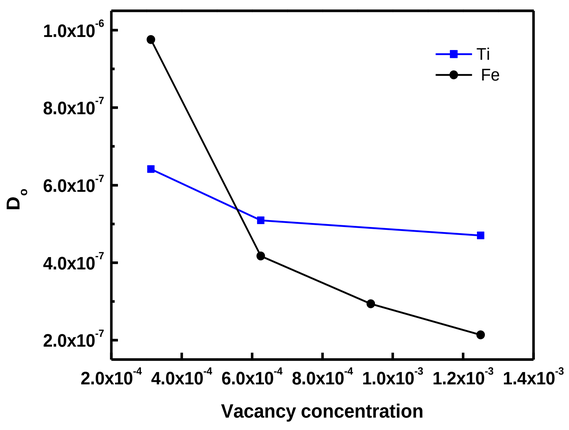
Effect of Titanium





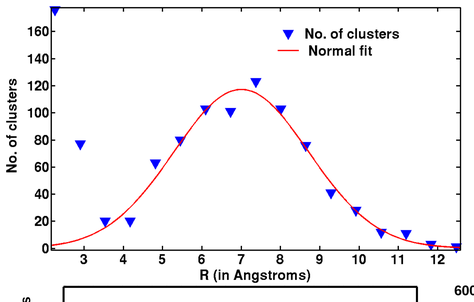
Diffusion coefficients of solute atoms





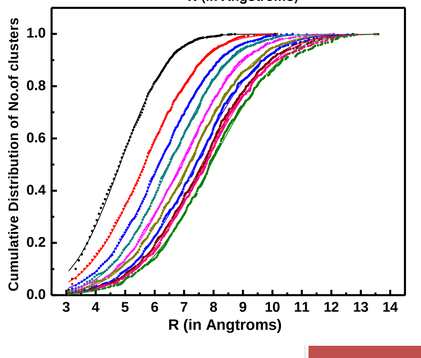
The diffusion coefficients of solute atoms in bcc Fe calculated using LKMC and compared with the diffusion coefficients calculated from first principles using Le Claire's nine frequency model and also the available experimental values.

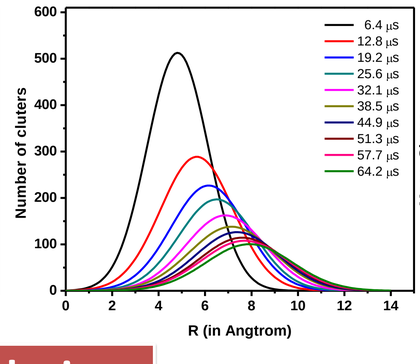
Size distribution of clusters

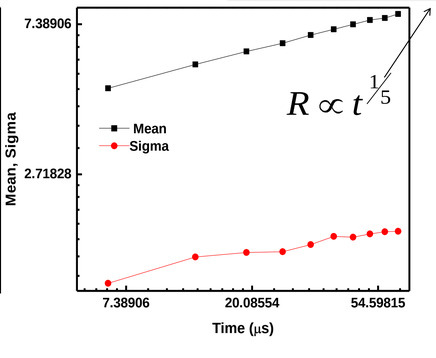


Normal distribution is found to give the best fit for the cluster size distribution (R >4 Å) out of Lognormal, Normal and gamma distributions. [ignoring the initial decaying portion(R < 4 Å) of size distribution].

Time exponent shows coagulation of clusters is the growth mechanism







Conclusions

- Mechanism of growth is the coagulation of the clusters.
- The Cluster Size follow a normal distribution.
- Presence of titanium reduces the size of clusters .

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