



Properties of vacancy clusters in FeMnNi alloys for the parameterization of OKMC models

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*IGRDM-19, Asheville NC
April 11th-15th 2016*

Properties of vacancy clusters in FeMnNi alloys for the parameterization of OKMC models

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^e EDF-R&D, Département Matériaux et Mécanique des Composants (France)

^f Vattenfall AB, Sweden

!!! PhD thesis on modeling of Mn-Ni-Si clusters in RPV steels !!!

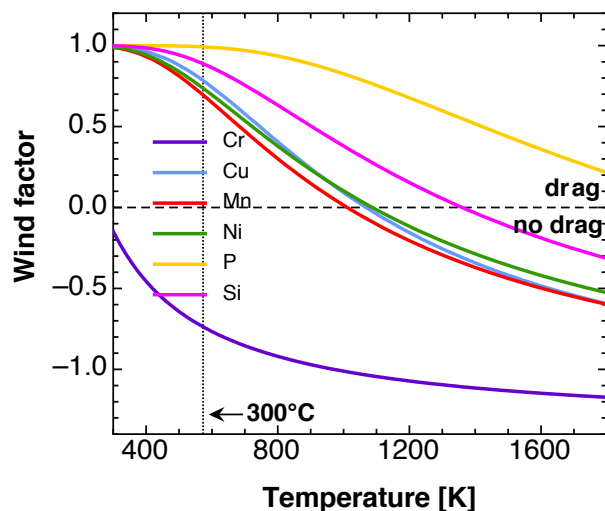
“Multiscale modeling of atomic transport phenomena in ferritic steels”

L. Messina, KTH Royal Institute of Technology (December 2015)

Asheville, April 12th 2016

Contact: messina@kth.se

Systematic vacancy drag at 300°C



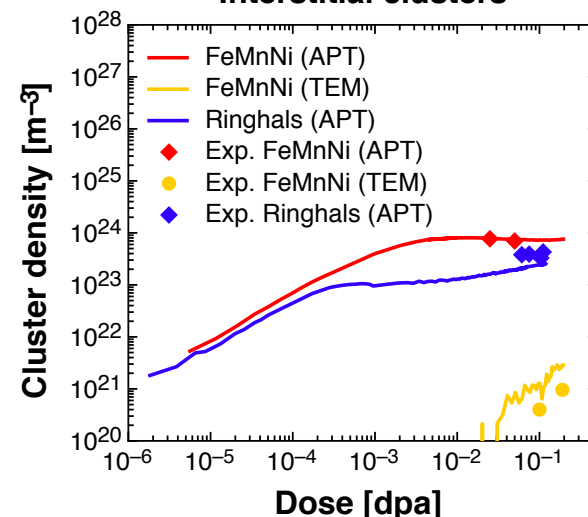
Solute-defect flux coupling in dilute alloys Fe(X), X = Cr, Cu, Mn, Ni, P, Si (and many more)

1. Solute transport by vacancy drag (Cu, Mn, Ni, P, Si) and single dumbbells (Cr, Mn).
2. Prediction of radiation-induced segregation profiles.
3. Effect of strain fields on solute transport next to dislocation lines.

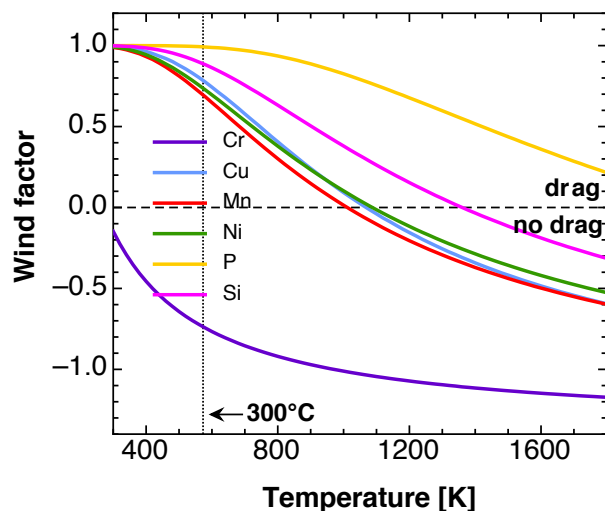
Modeling of solute transport in kinetic Monte Carlo (KMC) simulations

1. Properties of vacancy-solute clusters in FeMnNi alloys.
2. Prediction of energy barriers by DFT-aided artificial neural networks.
3. Microstructure evolution simulation of high-Mn, high-Ni RPV steels (Ringhals).

Interstitial loops $\Leftrightarrow$ MNSPs Interstitial clusters



Systematic vacancy drag at 300°C



Solute-defect flux coupling in dilute alloys Fe(X), X = Cr, Cu, Mn, Ni, P, Si (and many more)

PRESENTED AT IGRDM-18

1. Solute transport by vacancy drag (Cu, Mn, Ni, P, Si) and single dumbbells (Cr, Mn).
2. Prediction of radiation-induced segregation profiles.
3. Effect of strain fields on solute transport next to dislocation lines.

Modeling of solute transport in kinetic Monte Carlo (KMC) simulations

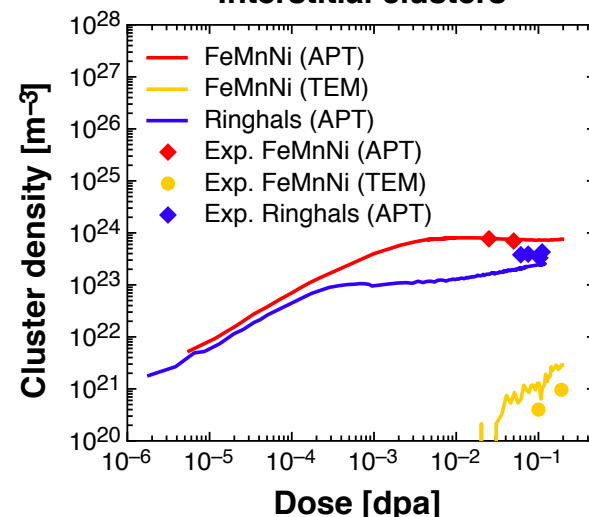
This presentation

1. Properties of vacancy-solute clusters in FeMnNi alloys.
2. Prediction of energy barriers by DFT-aided artificial neural networks.
3. Microstructure evolution simulation of high-Mn, high-Ni RPV steels (Ringhals).

Lorenzo's presentation

Interstitial loops $\Leftrightarrow$ MNSPs

Interstitial clusters



- Objective: parameterization of object KMC simulations of RPV microstructure evolution.
- Two alloys: model Fe-C-MnNi alloy^[1] and Ringhals RPV steel^[2].
- Parameterization of all objects.

MOBILITY

Probability of migration*

STABILITY

Probability of dissociation

Size	Pref ^{mig}	E ^{mig}	Pref ^{diss}	E ^{diss}
1	8.1e13	0.31 eV	-	-
2	3.4e14	0.42 eV	6e12	0.30 eV
3	1.2e13	0.42 eV	6e12	0.30 eV
4	1.2e13	0.80 eV	6e12	0.30 eV
5	1.6e12	0.10 eV	6e12	0.30 eV
...	...	...	...	...

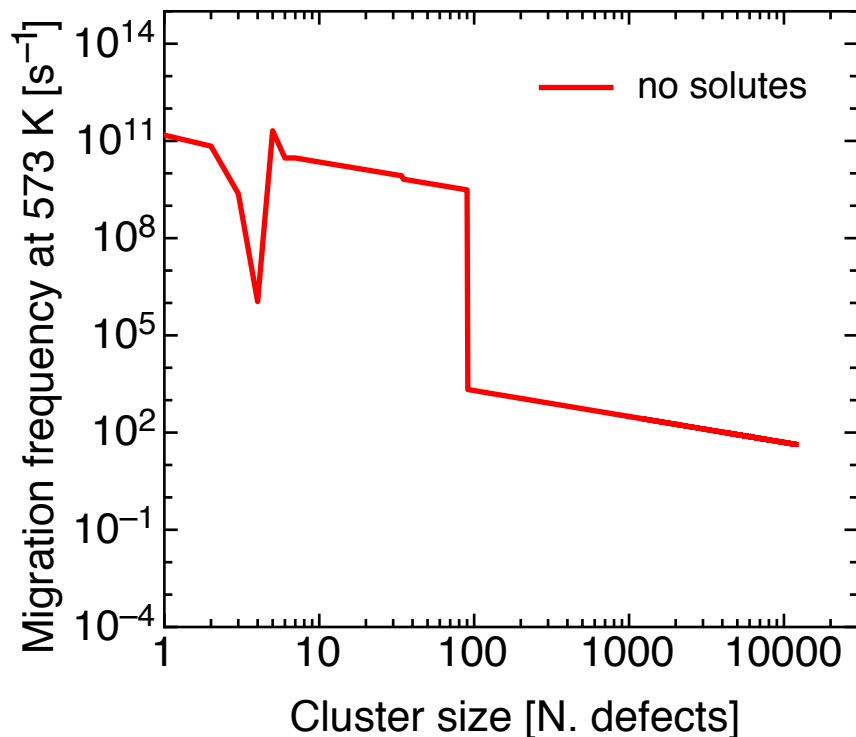
- Solutes can be introduced **explicitly** or with a “gray-alloy” approach.
- Usual techniques: kinetic Monte Carlo, molecular dynamics, ab initio with mean-field treatment.

[1] M. Hernández-Mayoral *et al.*, J. Nucl. Mat. **399** (2010).

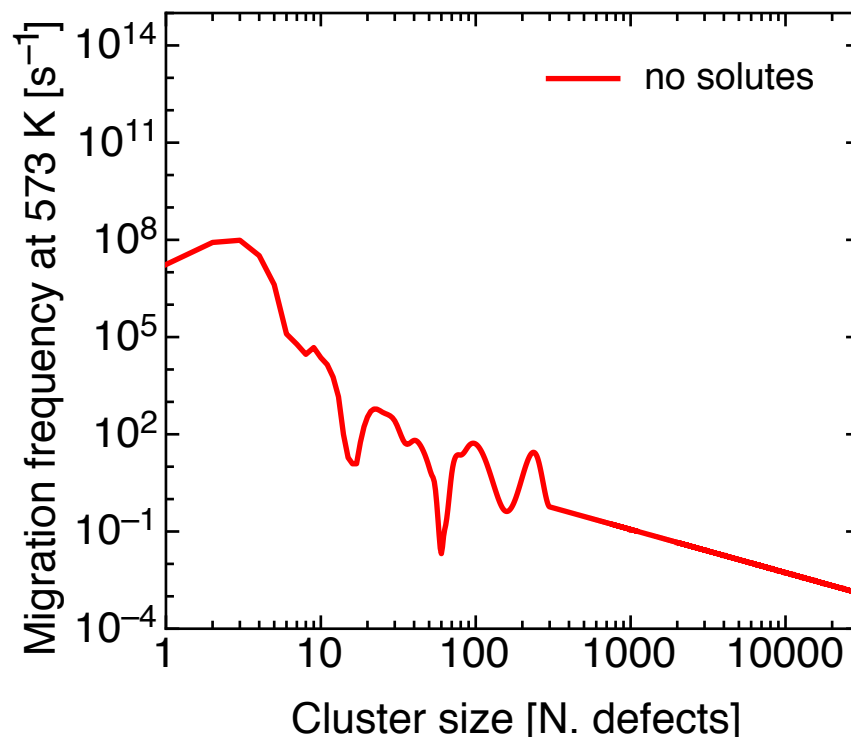
[2] P. Efsing *et al.*, J. ASTM Int. **4** (2007).

V. Jansson *et al.*, J. Nucl. Mat. **443** (2013)

INTERSTITIALS



VACANCIES



D. Terentyev *et al.*, Phys. Rev. B **75** (2007)

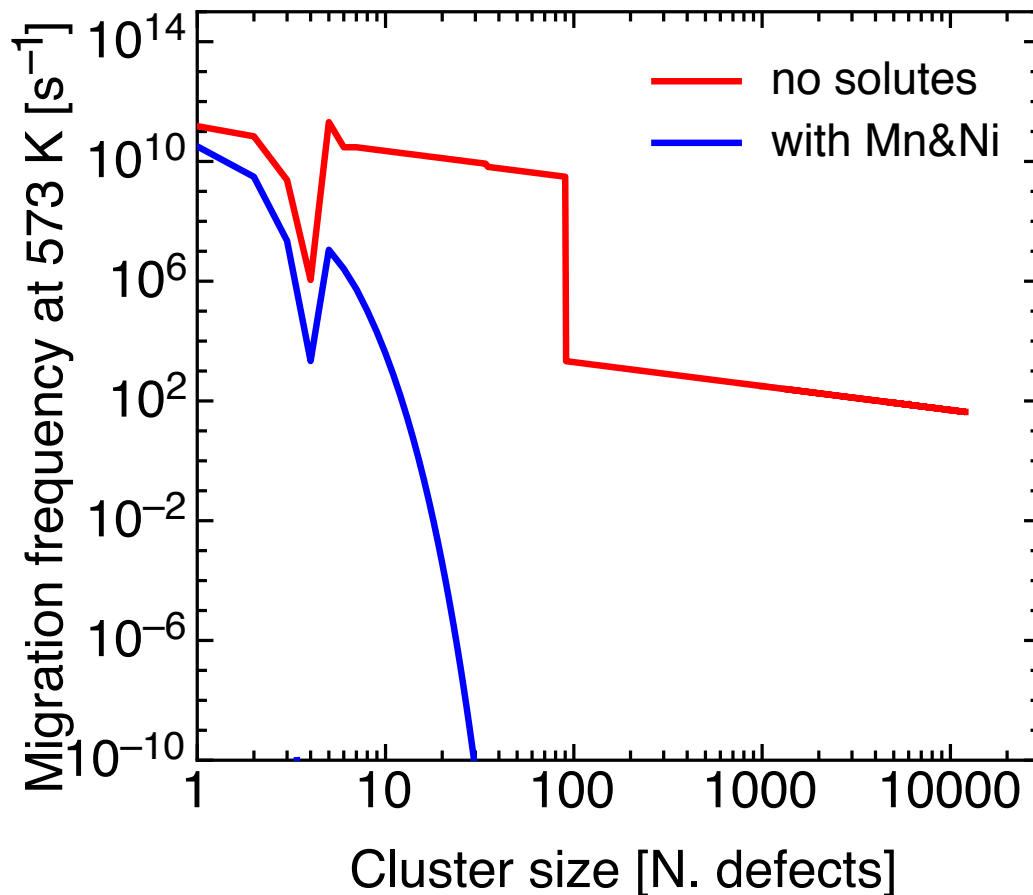
N. Anento *et al.*, Mod. Sim. Mat. Sci. Eng. **18** (2010)

- Molecular dynamics simulations.
- Postulated substantial slowdown for $n >$

N. Castin *et al.*, J. Nucl. Mat. **429** (2012).

- Atomistic KMC simulations with neural network prediction of migration barriers, based on molecular dynamics database.

INTERSTITIALS



- Mobility reduction due to strong attractive interaction between interstitial clusters and Mn, Ni.
- In analogy to effect of Cr on interstitial clusters in Fe^[1].

$$D_n^{\text{FeMn}}$$

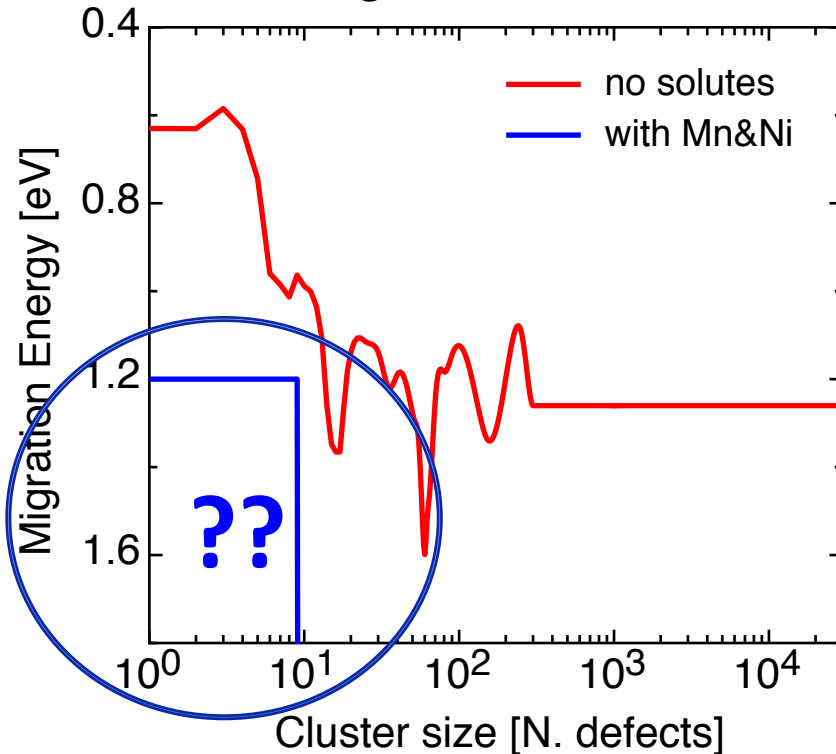
Cluster-solute binding energy
(DFT calculations by C. Domain):

$$E_b^{\text{Mn}}$$

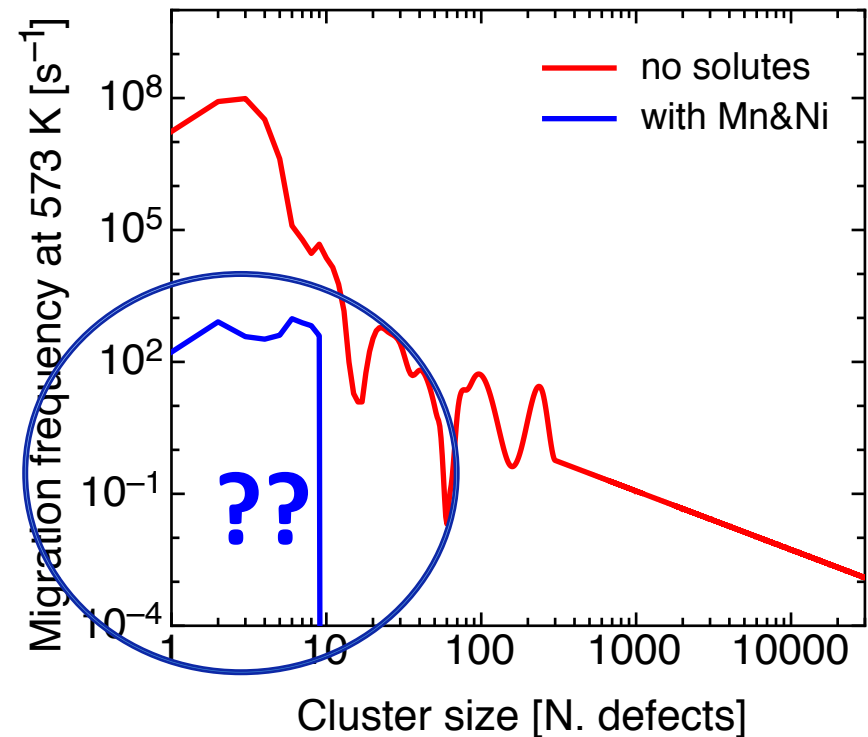
^[1] D. Terentyev *et al.*, Philos. Mag. Lett. **85** (2005)

VACANCIES

Migration barriers

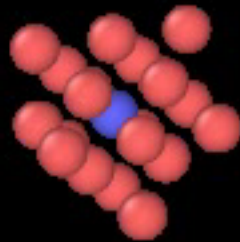


Migration frequency



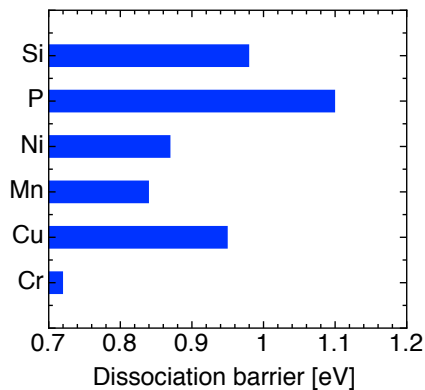
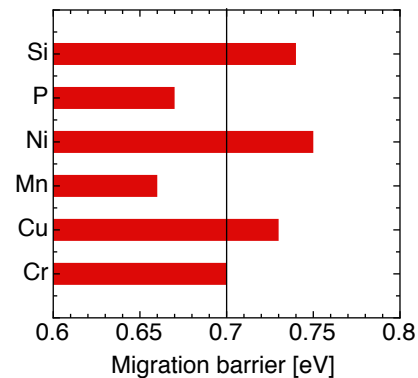
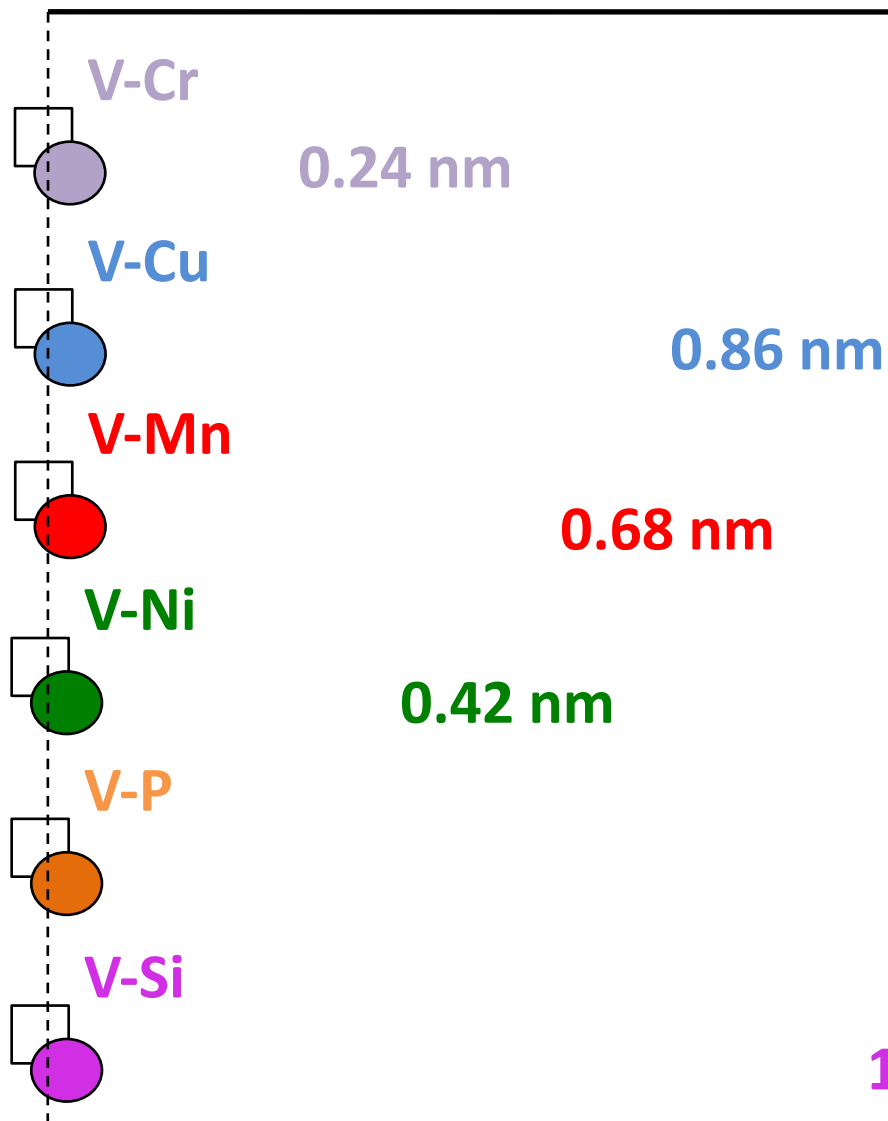
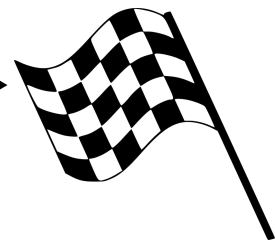
- “Arbitrary” reduction of vacancy cluster mobility (and immobilization for $n > 10$) to match experimental characterization of FeMnNi alloy.
- Same assumption works also for Ringhals steels (Lorenzo’s previous presentation).
- Possible explanations: effect of Mn/Ni solutes OR vac-Mn-Ni interaction with carbon traps.

Atomistic KMC method



Vacancy-solute pairs

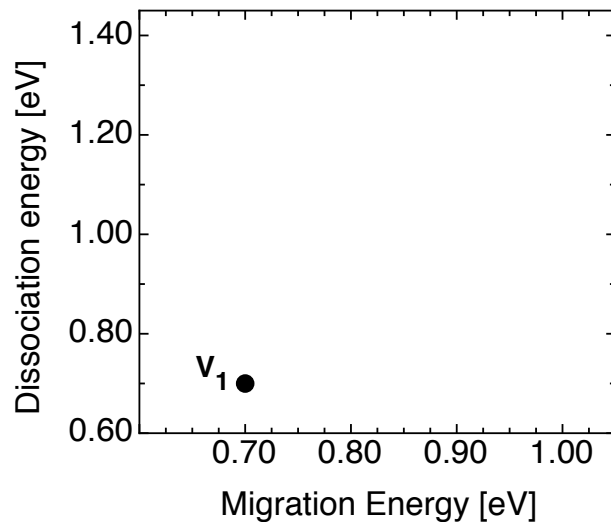
MEAN FREE PATH BEFORE DISSOCIATION (550 K)



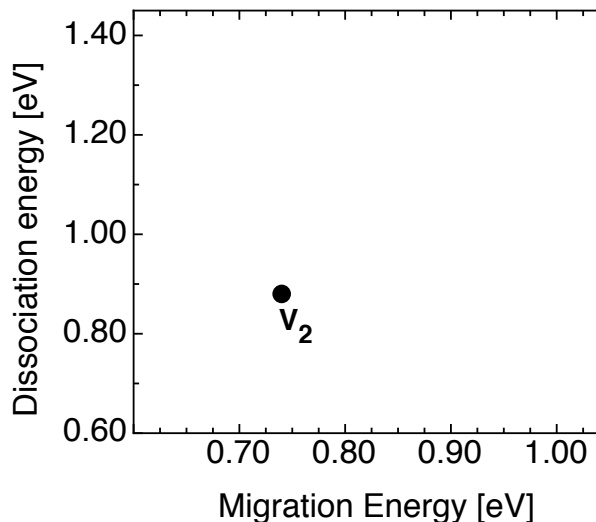
FROM AB INITIO DATA!!

Mobility of $V_xMn_yNi_z$ clusters

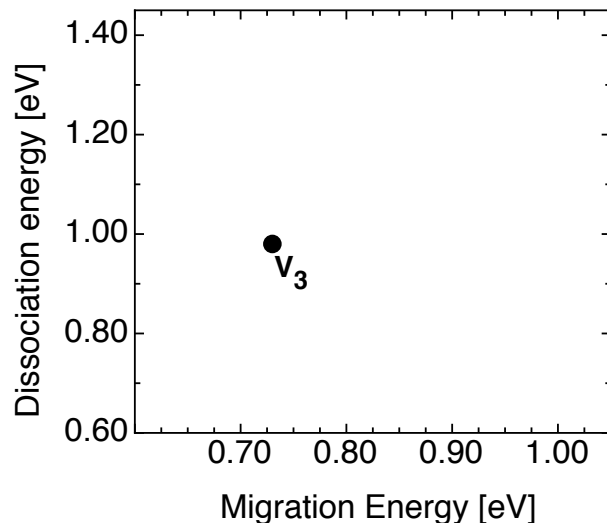
1-vacancy clusters



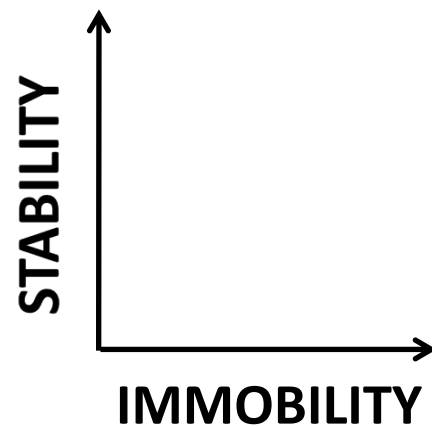
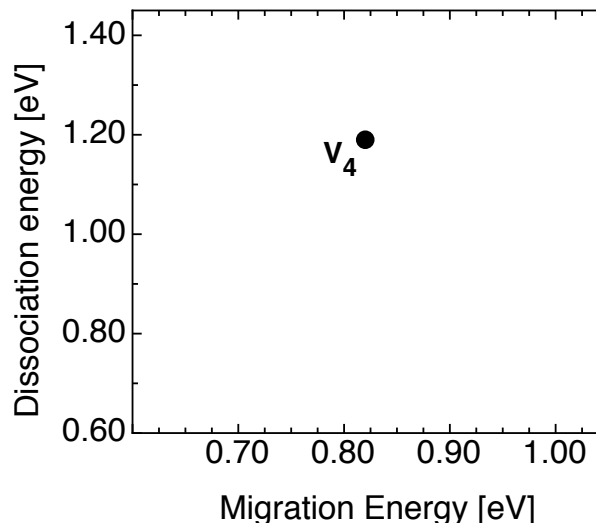
2-vacancy clusters



3-vacancy clusters

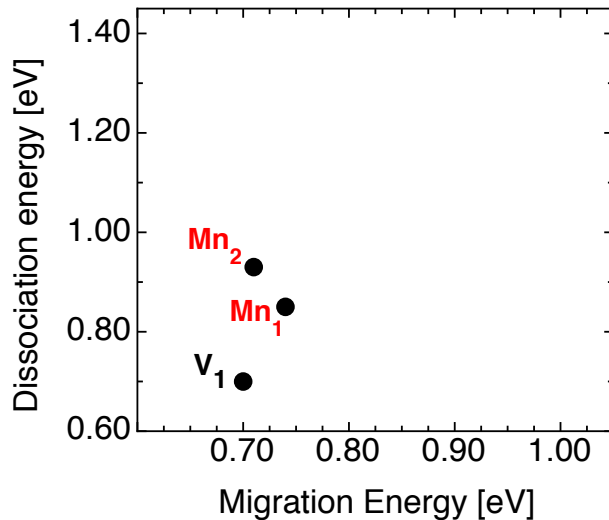


4-vacancy clusters

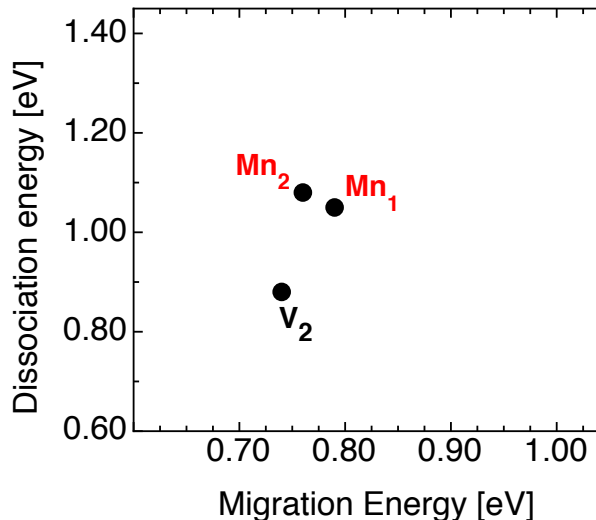


Mobility of $V_xMn_yNi_z$ clusters

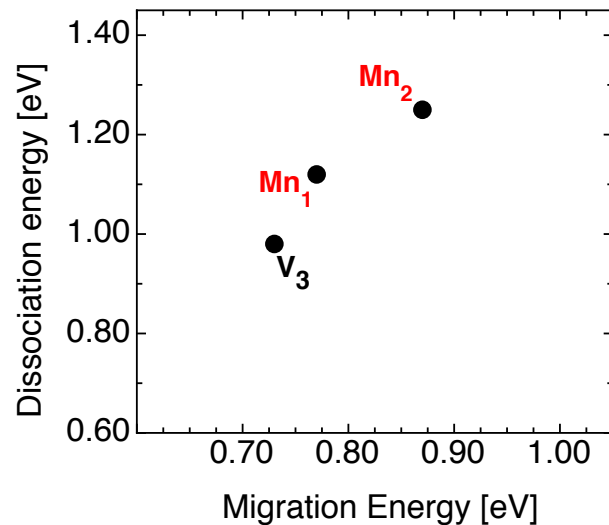
1-vacancy clusters



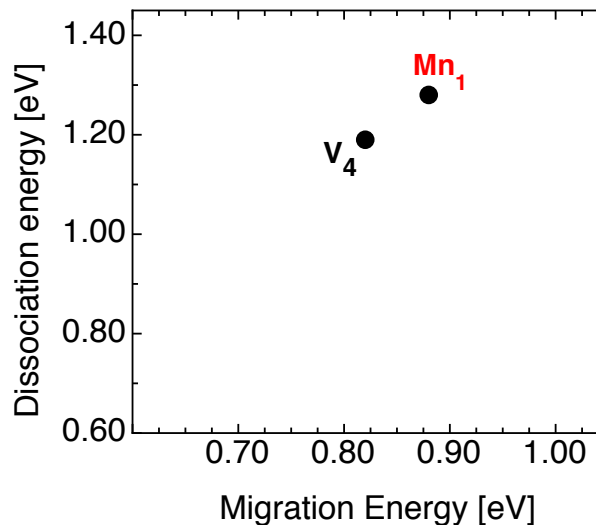
2-vacancy clusters



3-vacancy clusters



4-vacancy clusters

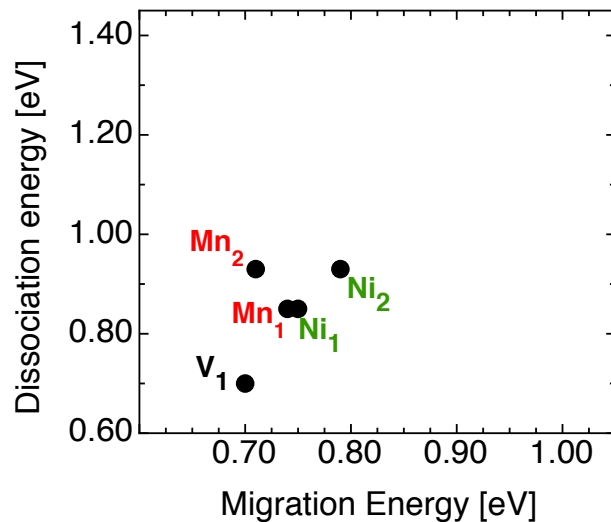


STABILITY ↑

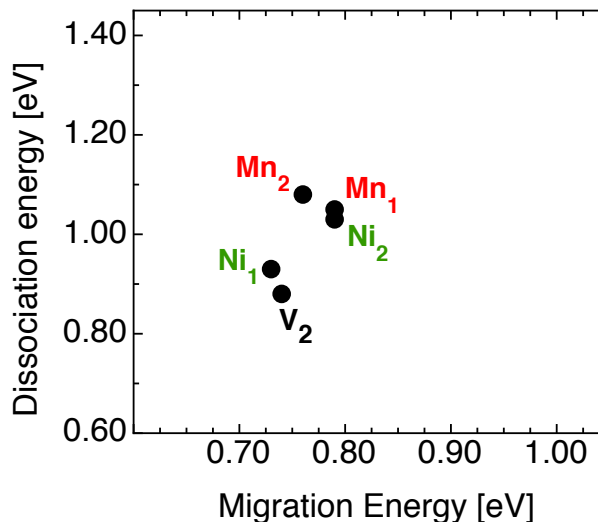
IMMOBILITY →

Mobility of $V_xMn_yNi_z$ clusters

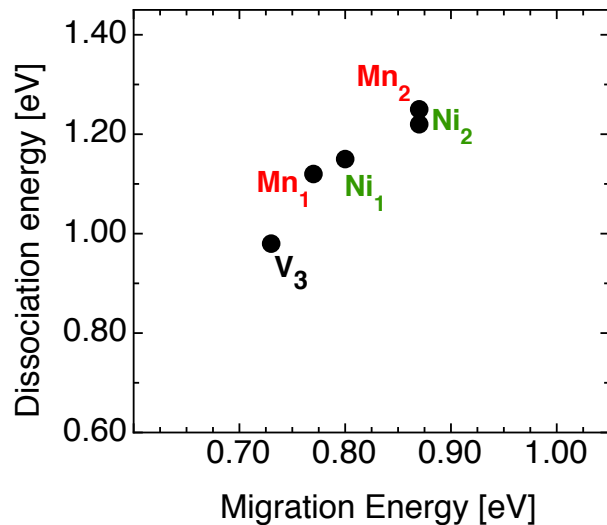
1-vacancy clusters



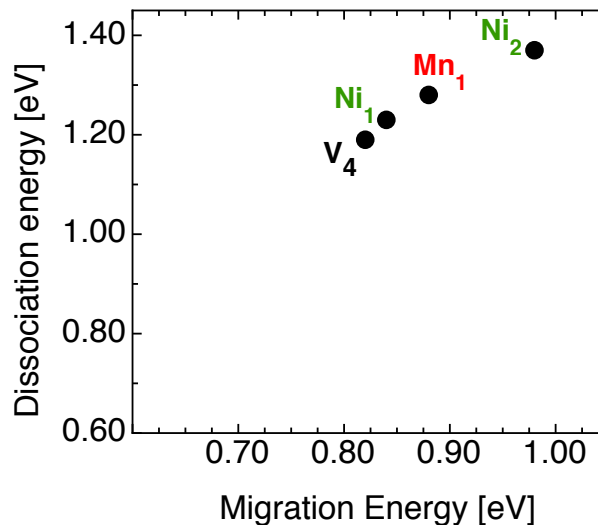
2-vacancy clusters



3-vacancy clusters



4-vacancy clusters

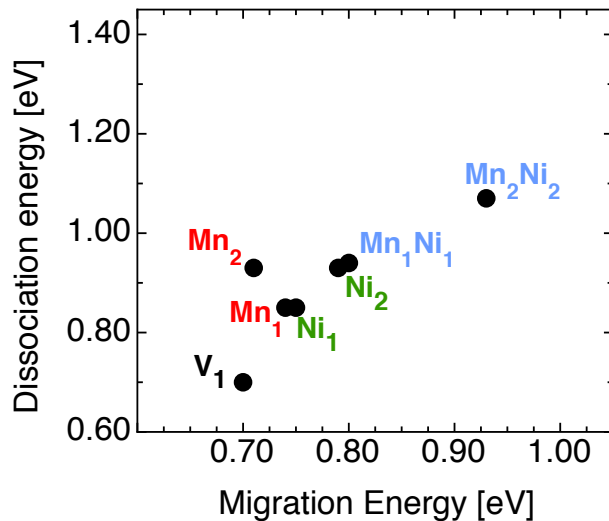


STABILITY ↑

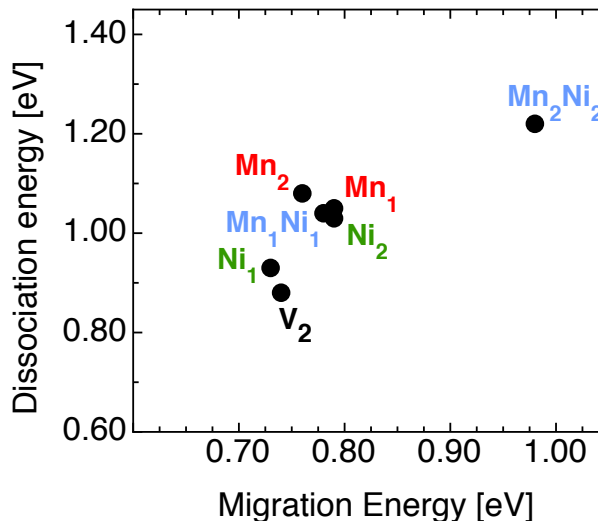
IMMOBILITY →

Mobility of $V_xMn_yNi_z$ clusters

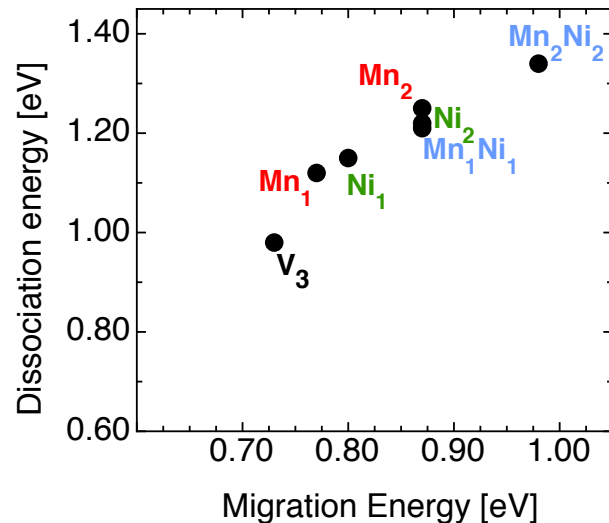
1-vacancy clusters



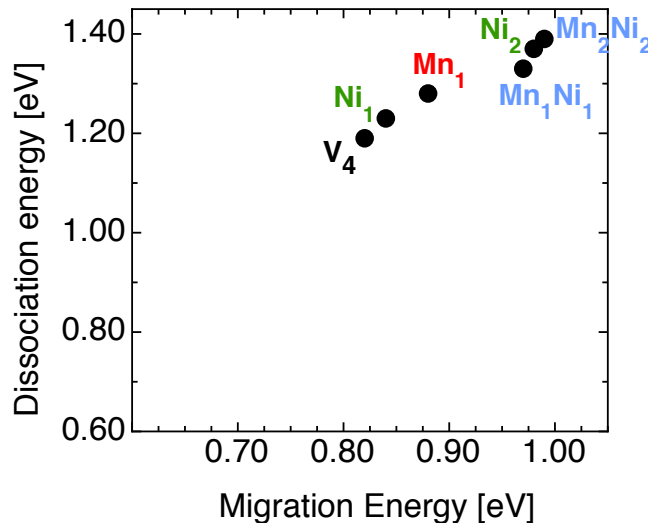
2-vacancy clusters



3-vacancy clusters



4-vacancy clusters

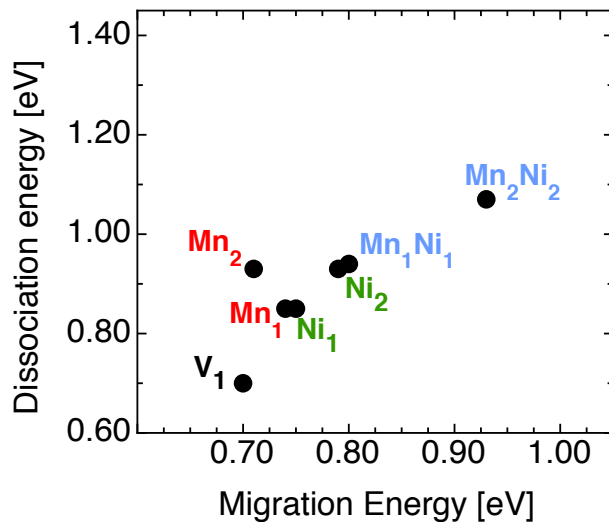


STABILITY ↑

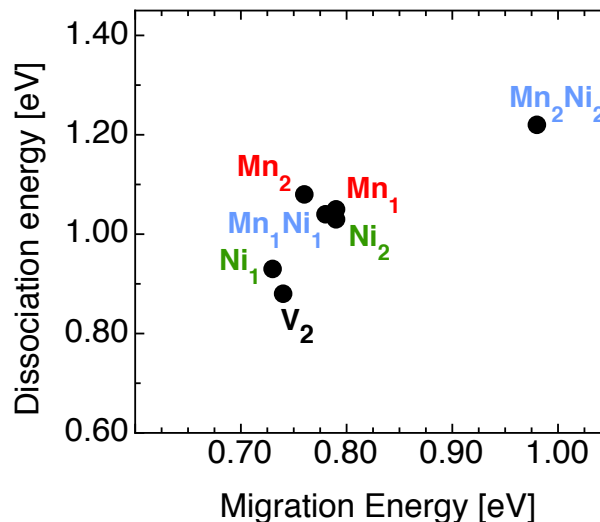
IMMOBILITY →

Mobility of $V_xMn_yNi_z$ clusters

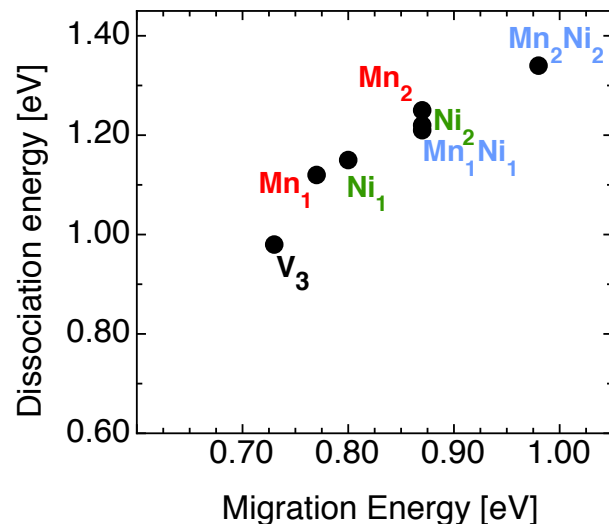
1-vacancy clusters



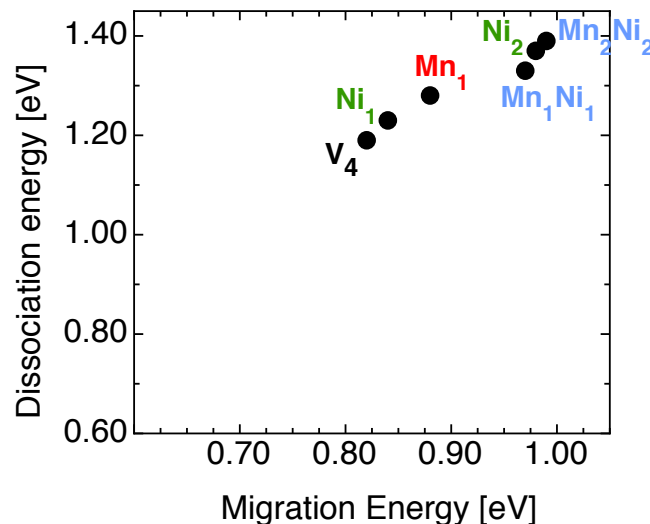
2-vacancy clusters



3-vacancy clusters

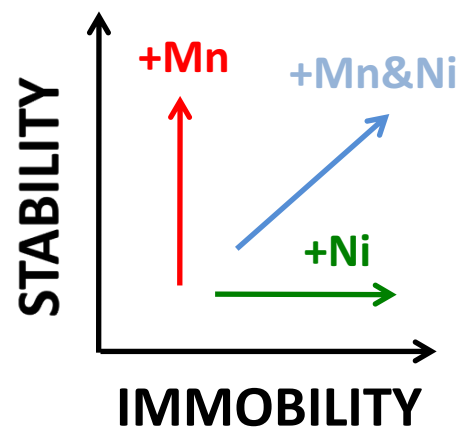


4-vacancy clusters

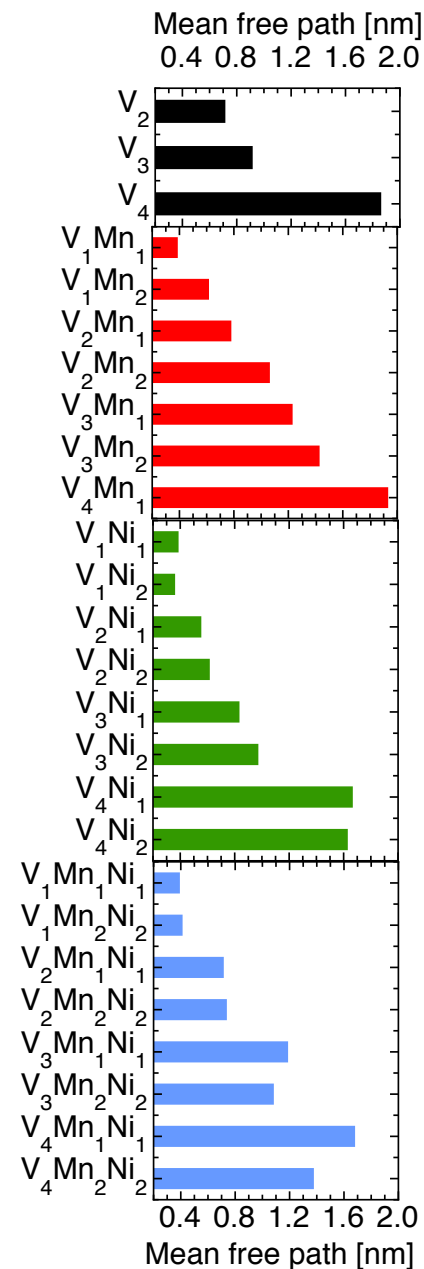
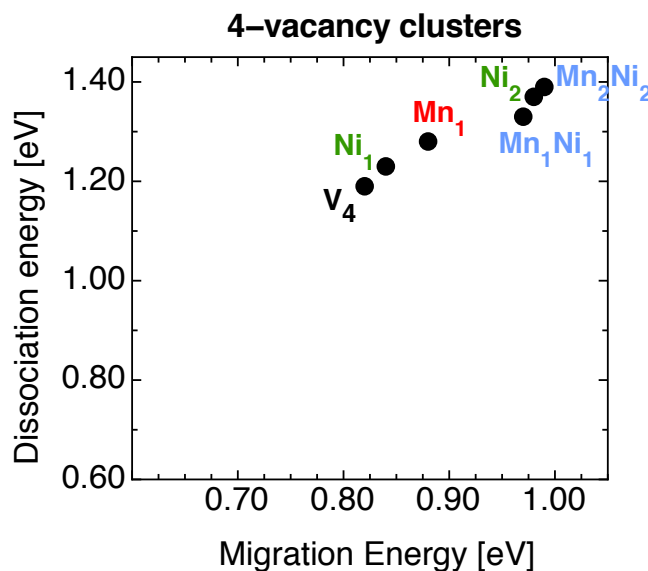
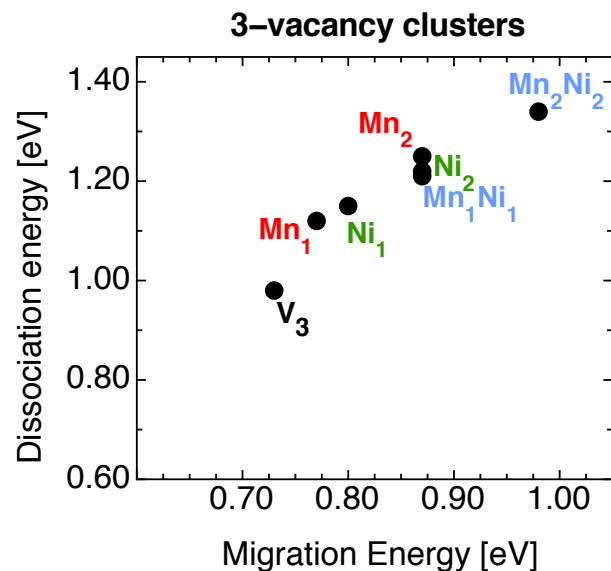
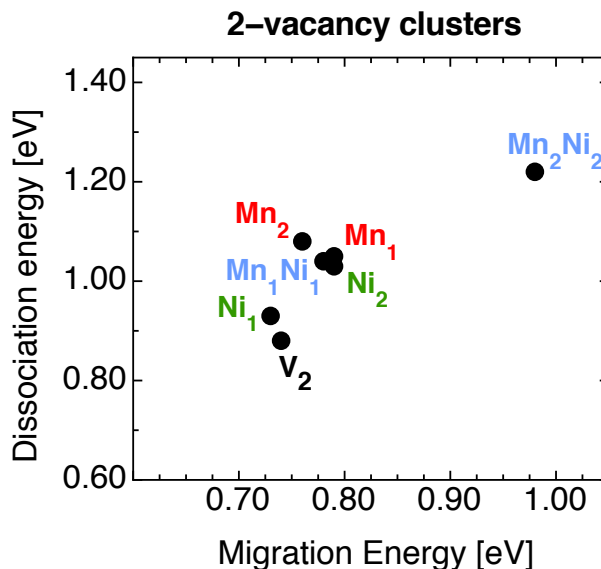
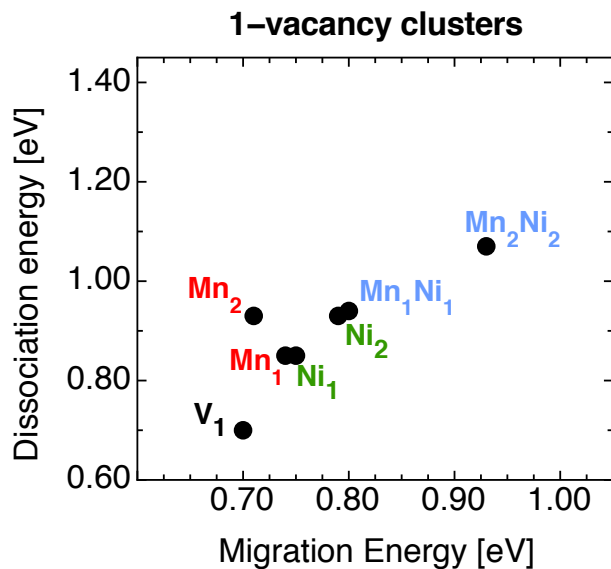


Partial
immobilization
observed

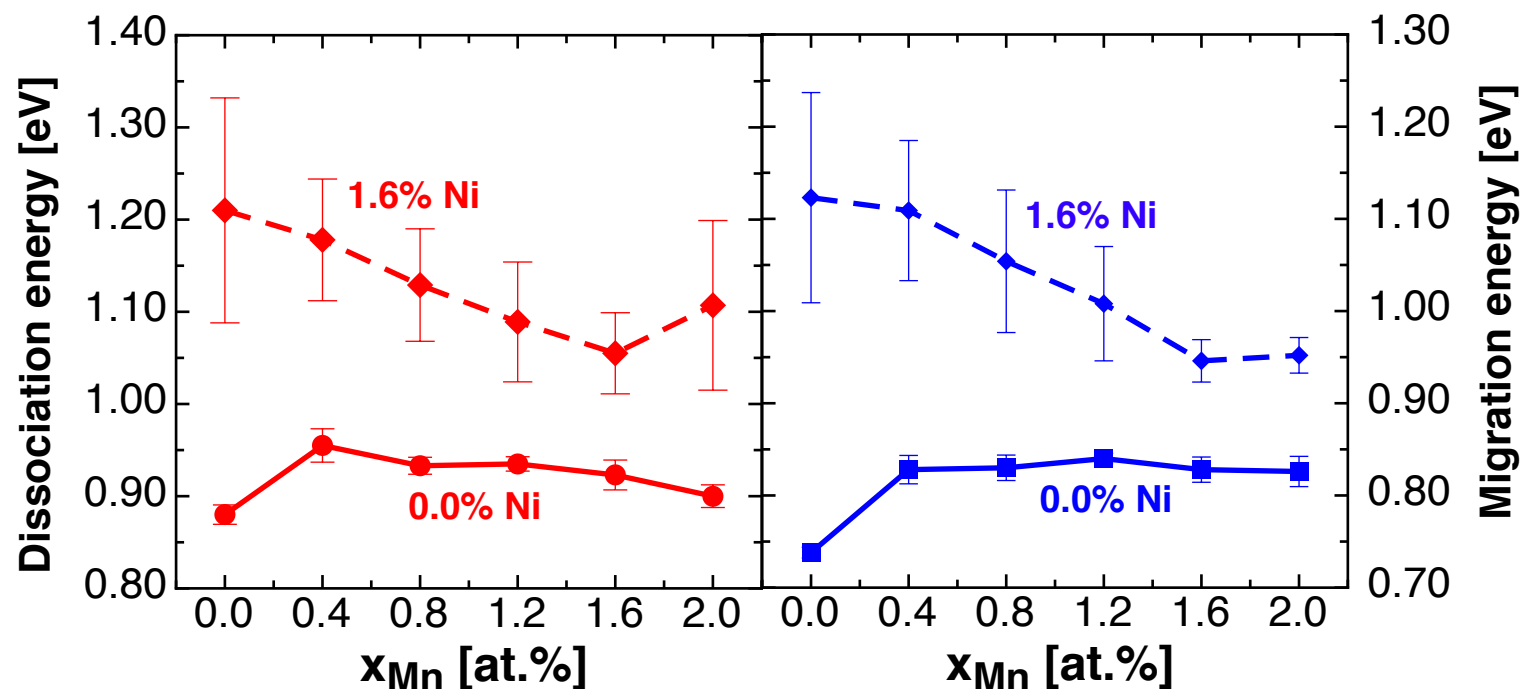
(Emig < 1.20 eV)



Mobility of $V_xMn_yNi_z$ clusters



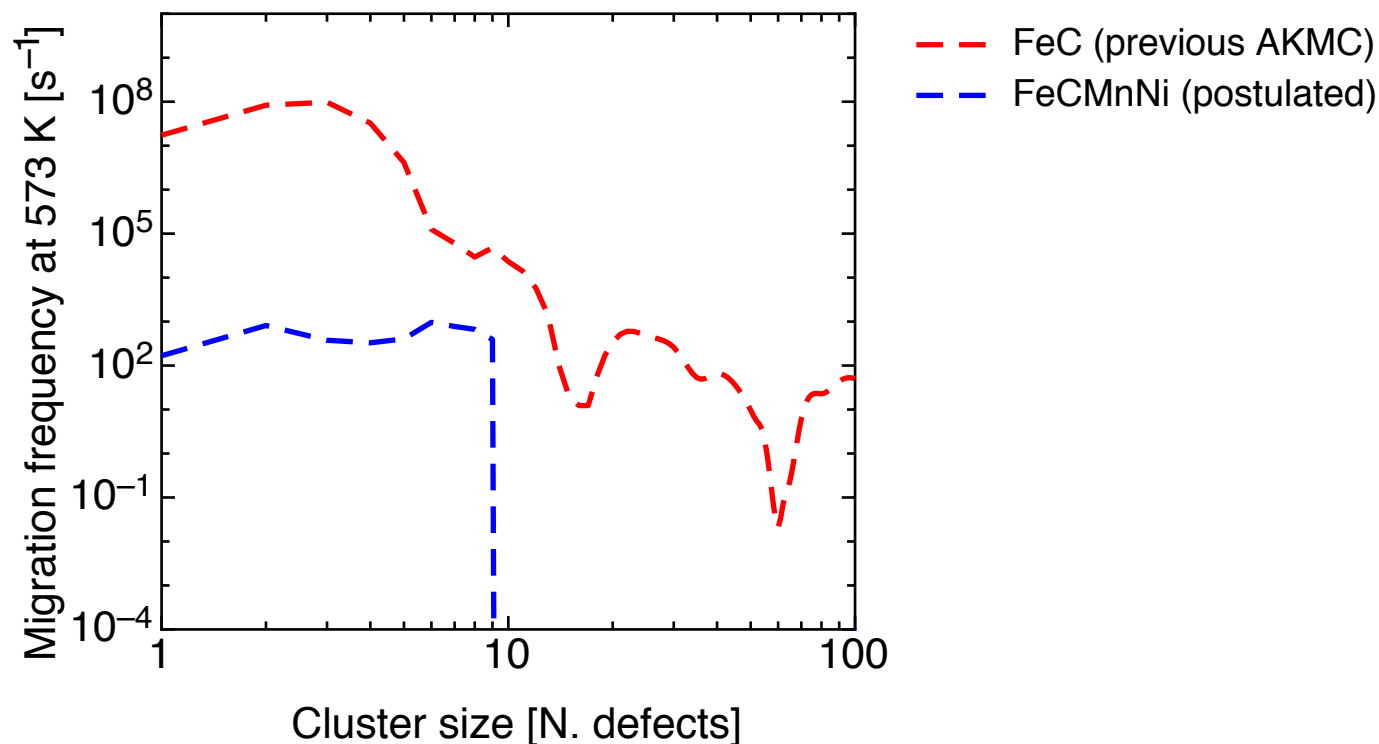
Stability and mobility of a di-vacancy in a random Fe-MnNi alloy



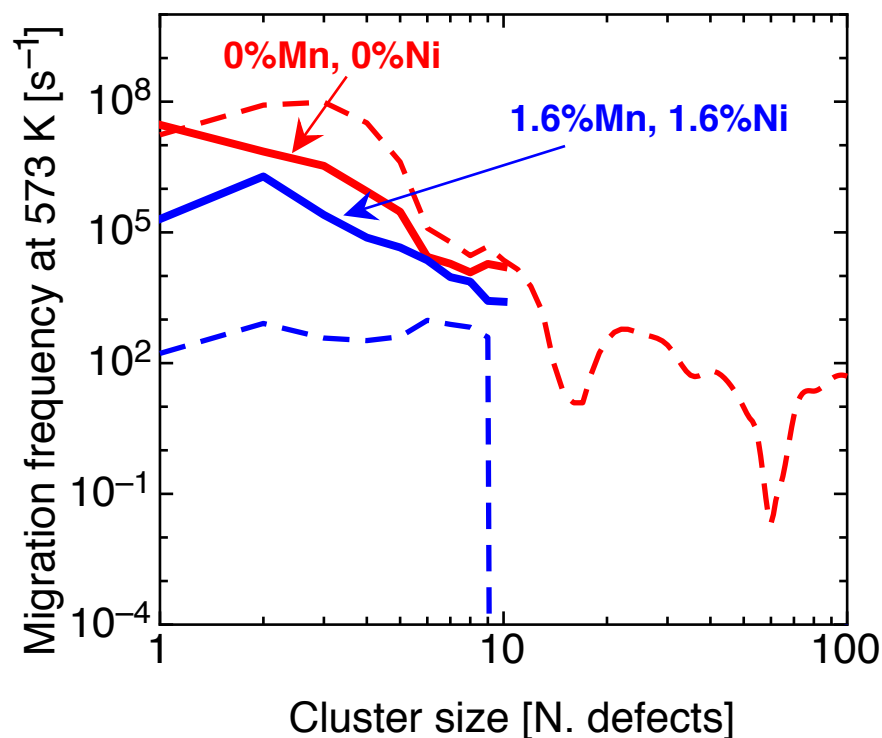
- Presence of Ni atoms has strong immobilizing effect.
- Presence of Mn atoms increases the probability of dissociation (because of strong V-Mn binding).
- Functions $E^{m/d} = f(x_{Mn}, x_{Ni})$ to be directly implemented in OKMC code.

VACANCY CLUSTERS

Migration frequency



VACANCY CLUSTERS Migration frequency



- FeC (previous AKMC)
- FeCMnNi (postulated)
- FeC (this AKMC)
- FeCMnNi (this AKMC)

- Estimated slowdown at 573 K is only 1 order of magnitude.

Conclusions

- The properties of vacancy clusters in FeMnNi were calculated by means of atomistic kinetic Monte Carlo simulations.
- Mn transport in Fe alloys is more efficient than Ni and Si.
- Mn seems to have a stabilizing effect on vacancy clusters, whereas Ni contributes more to the slowdown.
- The current calculations do not confirm a slowdown of vacancy clusters as strong as assumed by Lorenzo's OKMC model. Effect of vacancy-carbon(-solute) complexes?

THANKS FOR YOUR ATTENTION!

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Publications

- L. Messina, M. Nastar, T. Garnier, C. Domain, P. Olsson, *Exact ab initio transport coefficients in bcc Fe-X dilute alloys*, Physical Review B **90**, 104203 (2014).
- L. Messina, L. Malerba, P. Olsson, *Stability and mobility of small vacancy-solute complexes in Fe-MnNi and dilute Fe-X alloys: A kinetic Monte Carlo study*, Nuclear Instruments and Methods in Physics Research B **352**, 61-66 (2015).
- L. Messina, *Multiscale modeling of atomic transport phenomena in ferritic steels*, PhD Thesis, KTH Royal Institute of Technology (2015).
- L. Messina, M. Nastar, N. Sandberg, P. Olsson, *Systematic electronic-structure investigation of substitutional impurity diffusion and flux coupling in bcc iron*, accepted for publication in Physical Review B (2016).
- L. Messina, M. Chiapetto, P. Olsson, C. Becquart, L. Malerba, *An object kinetic Monte Carlo model for the microstructure evolution of neutron-irradiated reactor pressure vessel steels*, accepted for publication in Nuclear Instruments and Methods in Physics Research B (2016).

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- Host institutions: KTH, CEA, EDF, SCK-CEN.
- Collaborators:
 - M. Nastar, T. Garnier, F. Soisson, T. Schuler (CEA)
 - C. Domain (EDF)
 - N. Castin, L. Malerba, M. Chiapetto (SCK-CEN)
 - C. Becquart (Université de Lille)



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