Modelling static and dynamic strain ageing in FeC alloys

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Emmanuel Clouet, SRMP, CEA, France

Normand Mousseau, Univ. Montreal, Canada

Roberto Veiga, Helio Goldenstein, Univ. Sao Paulo, Brasil

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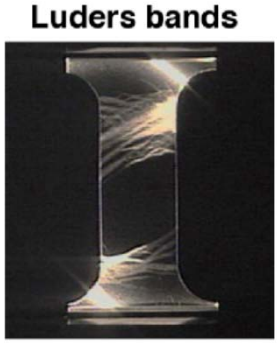
Project Capes-Cofecub:
PH 770 13

Objectives:

Understand the formation of Cottrell atmospheres, and the strain effect associated in FeC and FeMnC model steels.

Strain ageing effects in metallic alloys observed at the macroscopic scale but originate from physical phenomena arising at an atomic scale



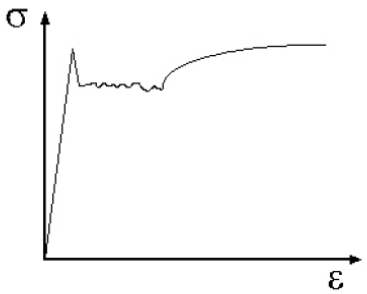


Figure I.1 : Courbe typique de traction avec palier de Lüders.

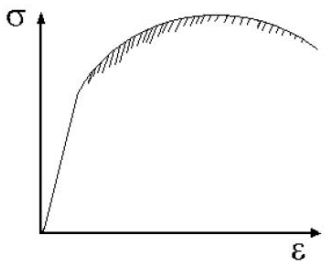
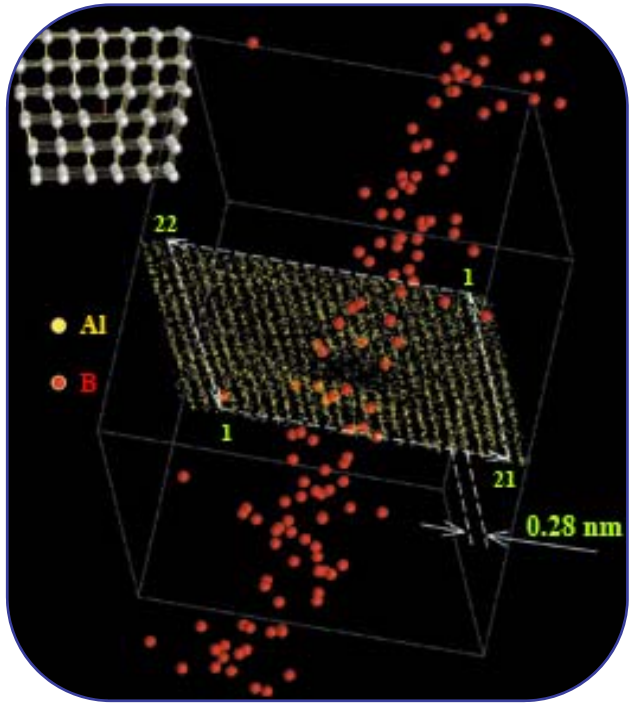


Figure I.2 : Courbe typique de traction avec hétérogénéités de Portevin - Le Chatelier.

PhD Belotteau, Centrale Paris, 2009



Cottrell atmosphere of boron atoms in the core of an edge dislocation in aluminium

D. Blavette *et al* / Science, 286 (1999) 2317

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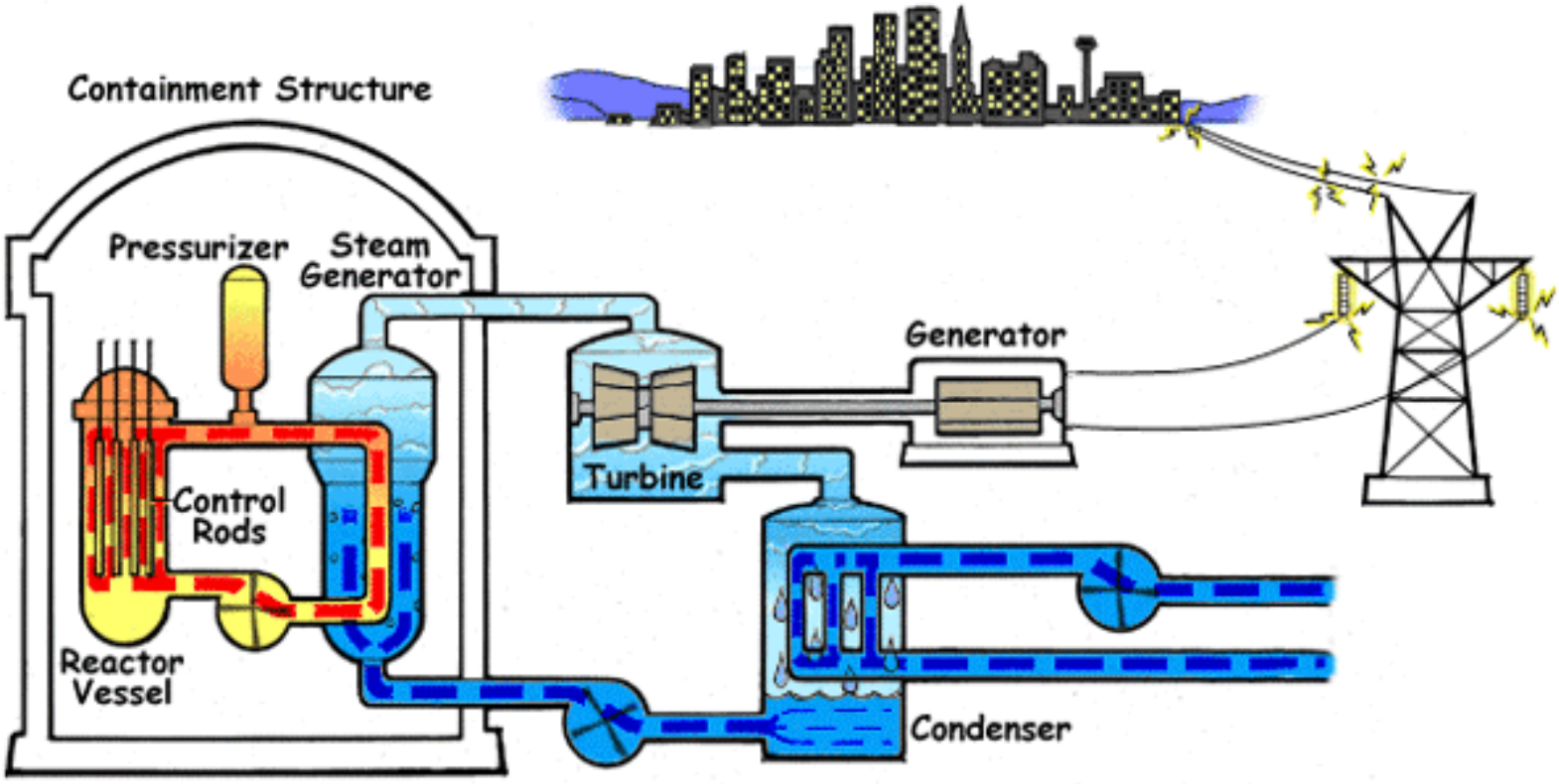
Understand the formation of Cottrell atmospheres, and the strain effect associated in FeC and FeMnC model steels.



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Cottrell and Bilby theory:

-Dislocations introduced by plastic deformation interact with interstitial C atoms ir solid solution through their respective stress fields.
==> carbon segregation to dislocations

-More C atoms segregate: an “atmosphere” grows around the dislocations.

-C Cottrell atmosphere hinders the dislocation motion upon reloading, such that a higher stress is required in order to make the dislocation tear away from the solutes.

Cottrell atmosphere formation = first stage of static strain aging. Second stage = carbide precipitation in the dislocation vicinity.

A. H. Cottrell and B. A. Bilby. Proc. Phys. Soc. A, 62 (1949) 49.

Hardening / softening behaviour of C atoms

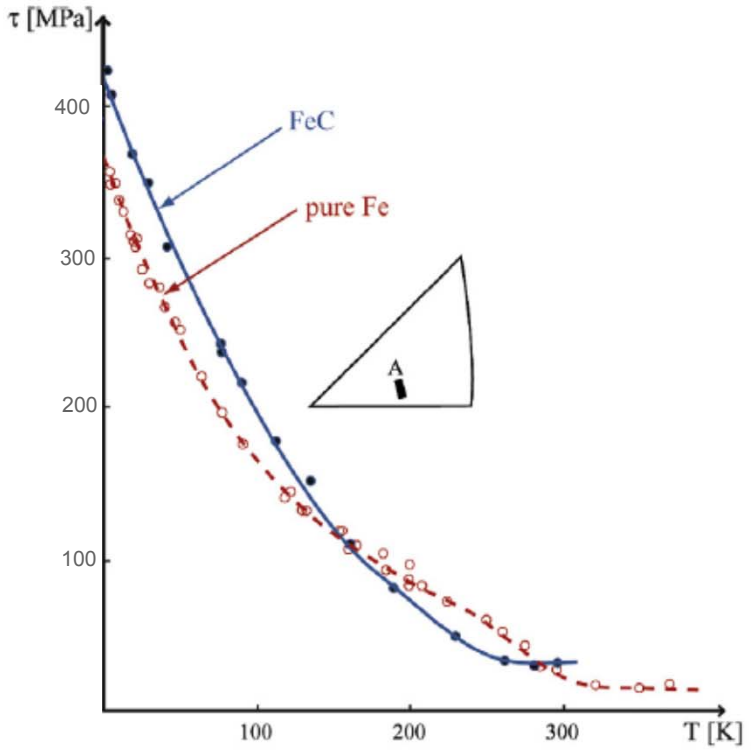

Fig. 1. Experimental activation area A and yield stress τ as functions of temperature T in Fe and FeC. The yield stress is taken as the resolved shear stress on the most stressed plane, and in a $\langle 1\,1\,1 \rangle$ direction (strain rate $1.7 \times 10^{-4}\,s^{-1}$). From Kuramoto et al. [6].

D. Caillard, Acta Mater. 59 (2011) 4974

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PhD Quoc Hoang Nguyen: atomic simulation of C- screw dislocation in Fe: impact on plasticity december 2009

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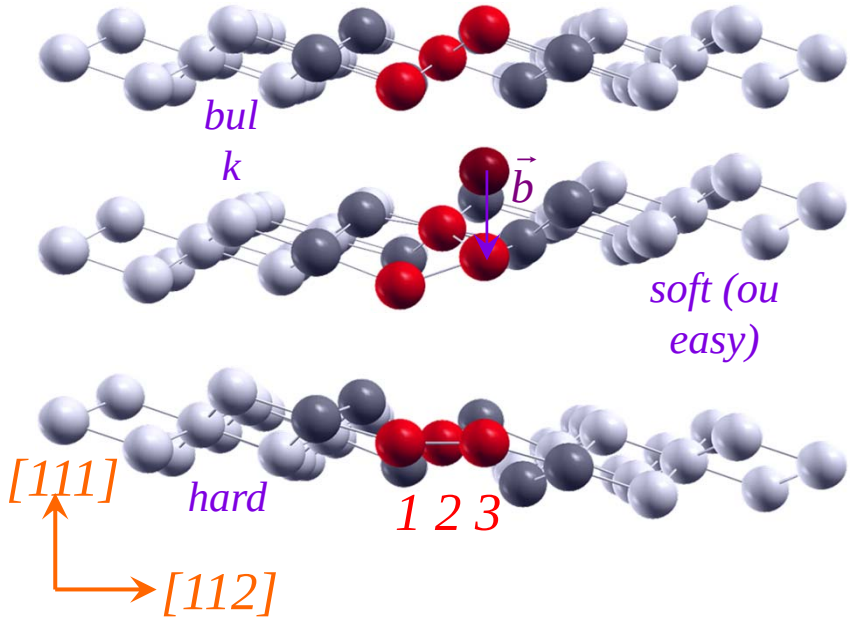
-One screw dislocation
-One C atom

FeC potential: predicts correctly screw disl. core configuration and E_{mig} C [Becquart]

soft (or easy) core: **stable.**
hard core: **métastable.**



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C.S. Becquart, J.M. Raulot, G. Bencteux, C. Domain, M. Perez, S. Garruchet, H. Nguyen, Comp. Mater. Sci **40** (2007) 119.
R. G. A. Veiga, C. S. Becquart, M. Perez, Comp. Mat. Sci. **82** (2014) 118

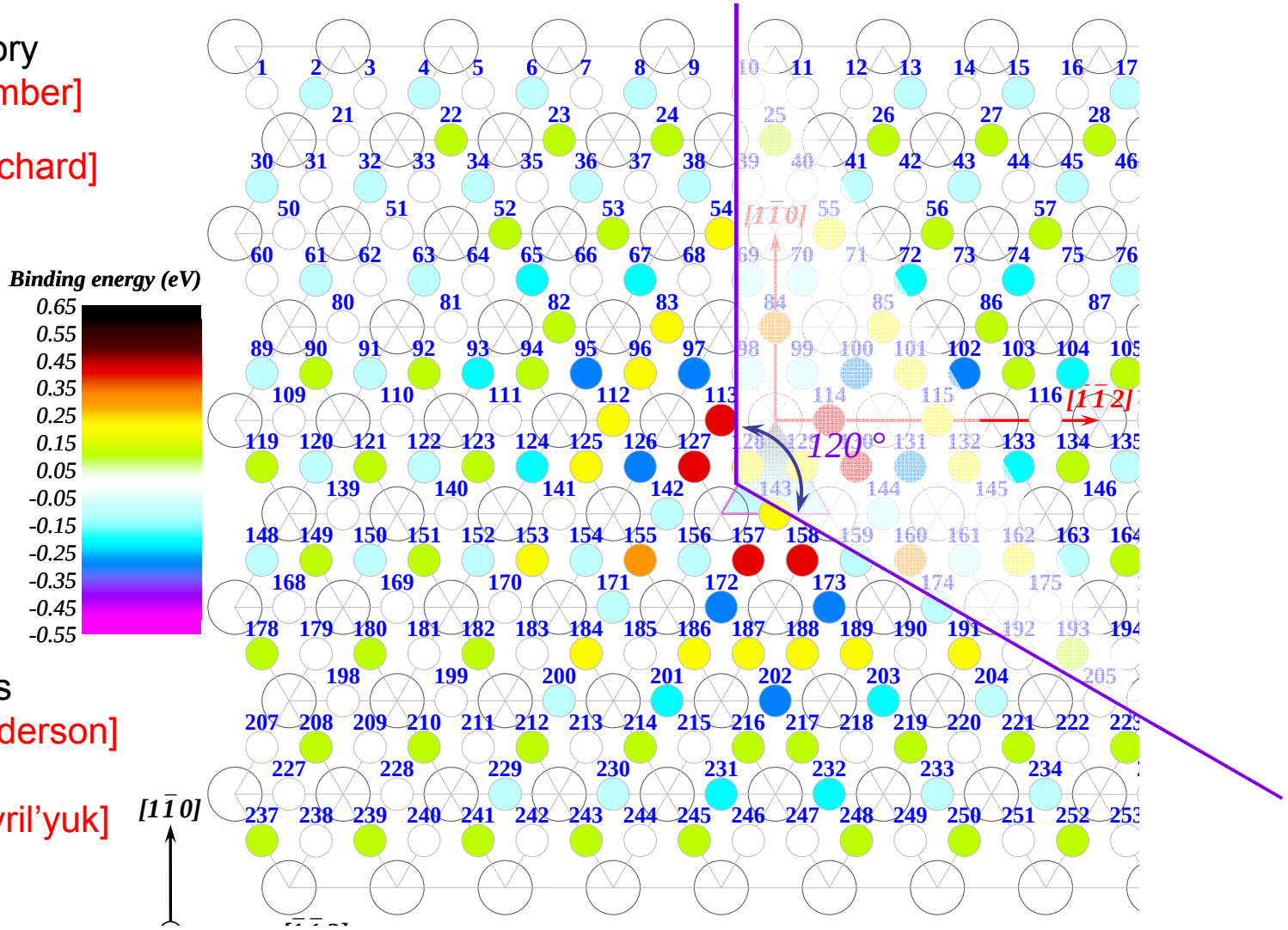
Binding energy between C and a screw dislocation

Elasticity theory
E_b = 0.5 eV [Kamber]

E_b = 0.70 eV [Cochard]

Experiments
E_b = 0.45 eV [Henderson]

E_b = 0.75 eV [Gavril'yuk]



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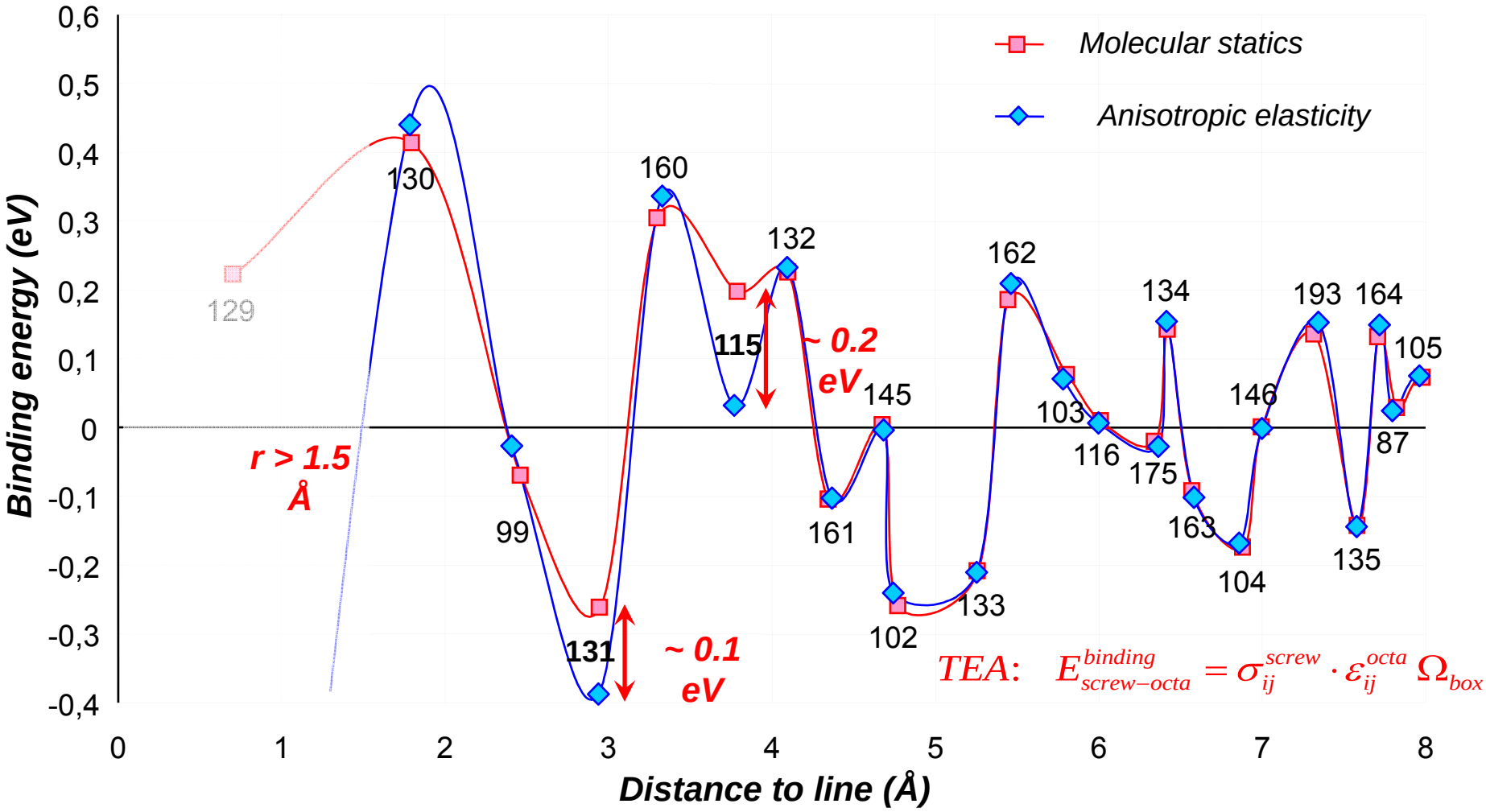
Kamber et al. *Acta Mater* **9** (1961) 403
Cochardt et al. *Acta Mater* **3** . (1955) 533
Gavril'yuk et al. Phys Met Metall 42 (1976) 1288.
B. Henderson B. Defects in crystalline solids. London: Edward Arnold:1972. p. 170.

Binding energy between C and a screw dislocation: Comparison with anisotropic elasticity theory



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E. Clouet, S. Garruchet, H. Nguyen, M. Perez & C. S. Becquart, Acta Mat. **56** (2008) 3450.

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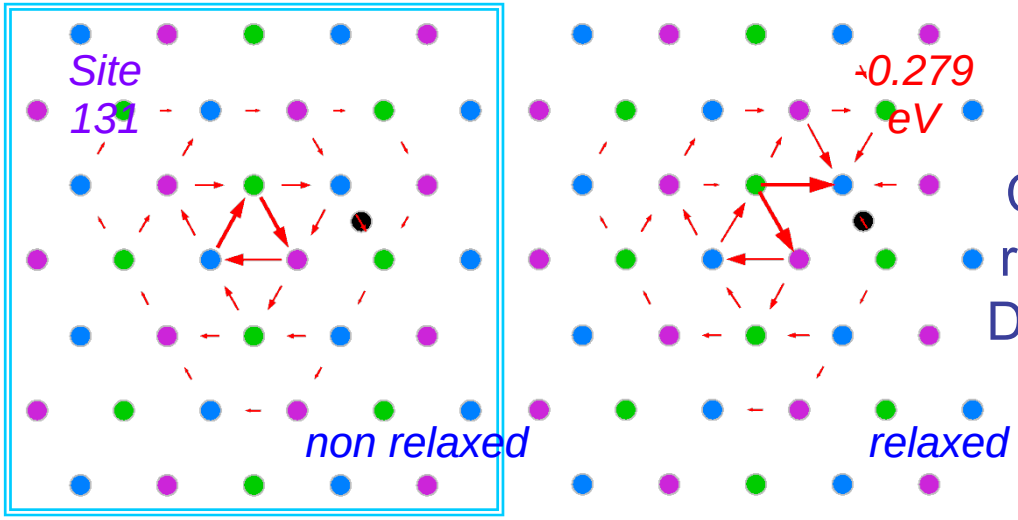
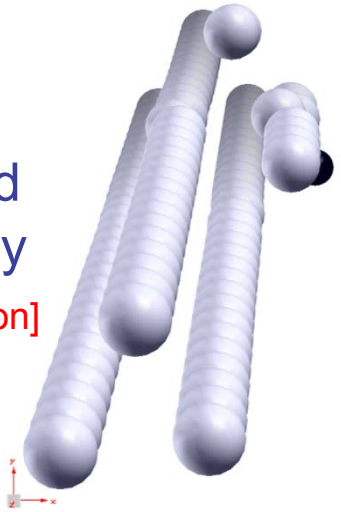
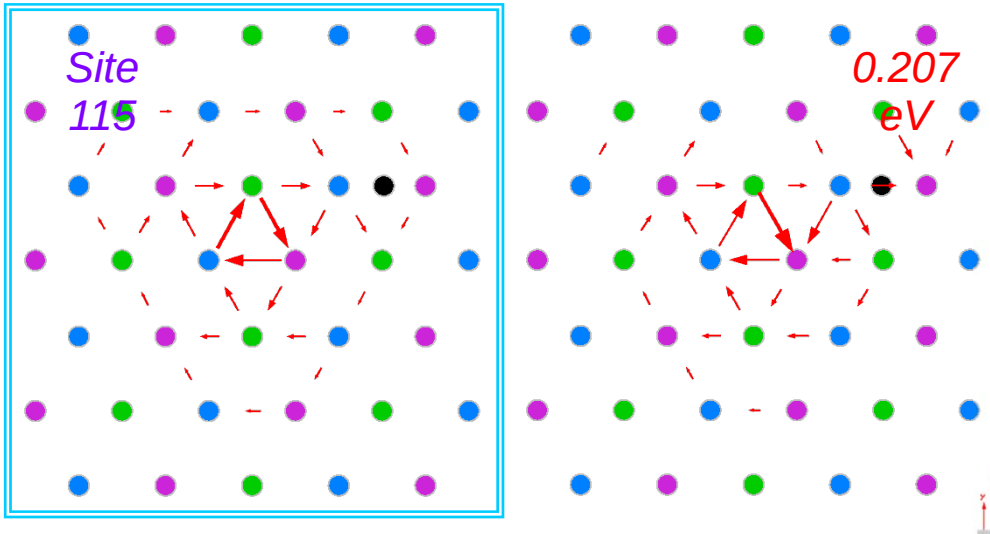
Disagreement with anisotropic elasticity theory

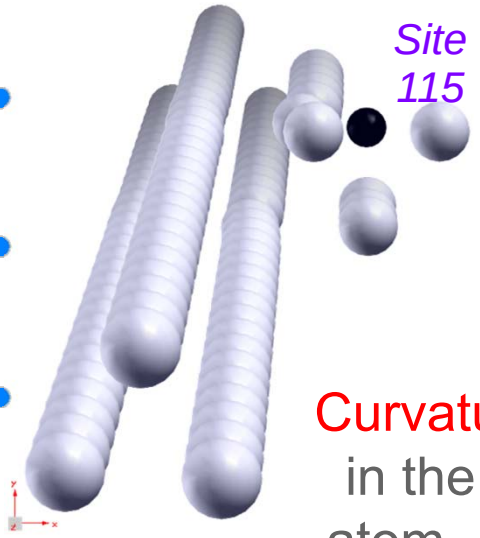


→ hard core. Confirmed recently by DFT [Ventelon]



Site
131





Site
115

Curvature of the line in the vicinity of C atom → local effect

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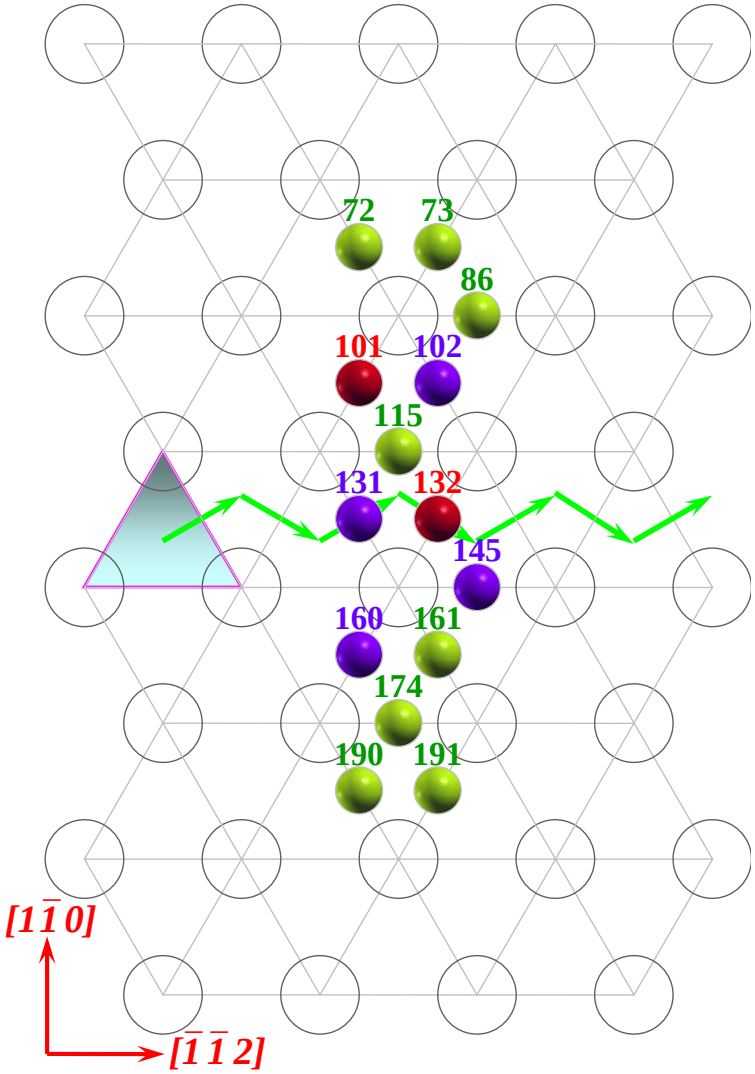
L. Ventelon, B. Luthi, E. Clouet, L. Proville, B. Legrand, D. Rodney, F. Willaime, Phys. Rev. B 91 (2015) 220102

Motion of dislocation facing a C atom



One screw dislocation and one C atom

3 behaviors:

C immobile, slip on {110} **C115**

C immobile, cross slip {112 } **C131**

C changes site, slip on {110} **C132**

- Critical shear stress decreases when T increases
- Dislocation pinning at low T (100K)
  → not observed at higher T (300 & 500 K)

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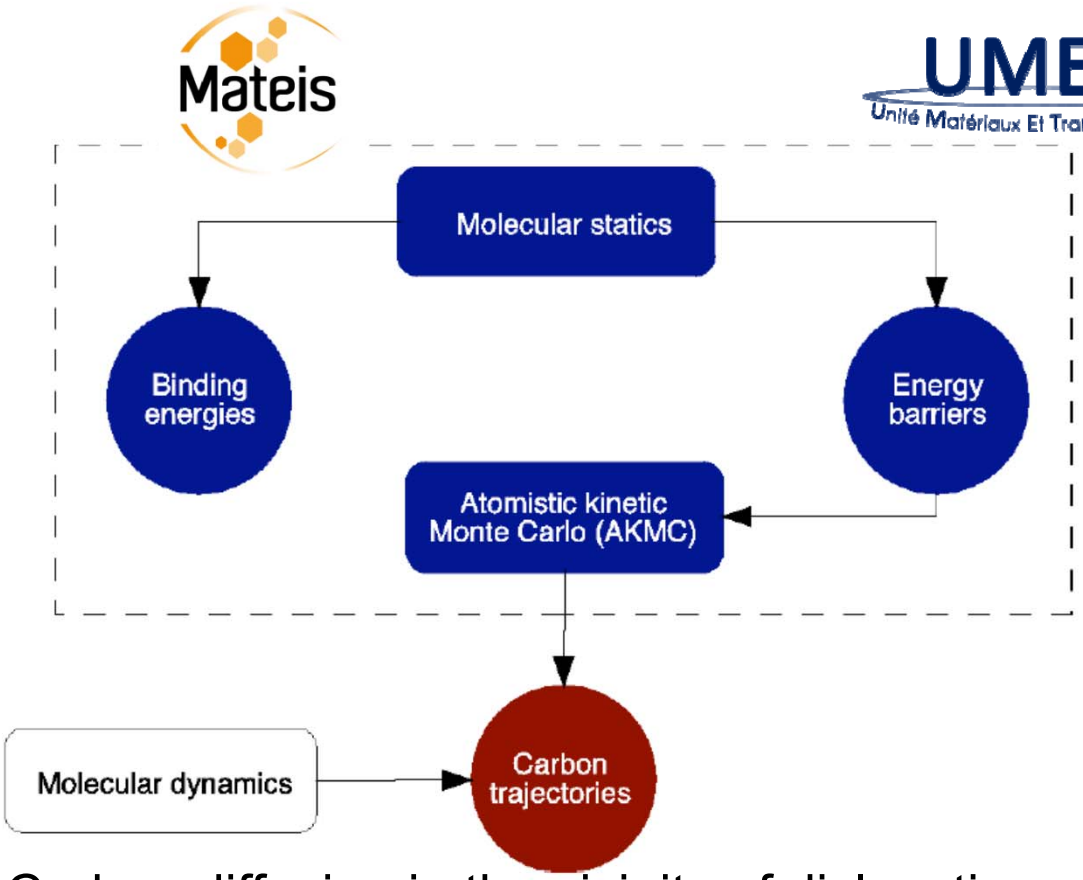
Roberto Veiga PhD thesis: september 2011: Computational insights into the strain aging phenomenon in bcc Fe at the atomic scale



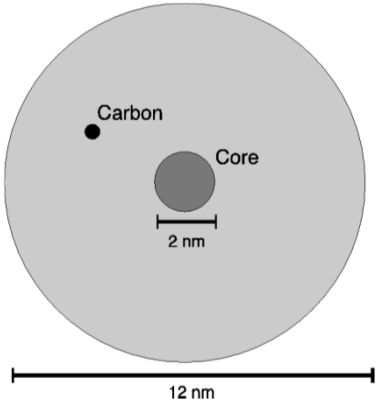
1/ Carbon diffusion in the vicinity of dislocations

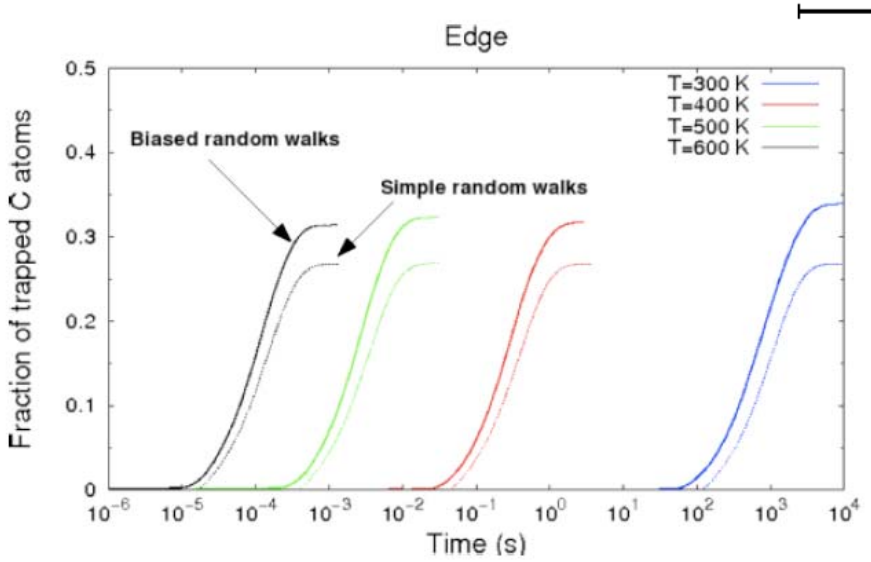
2/ Carbon diffusion in the core of a dislocation

3/ Carbon distribution in a Cottrell atmosphere

1/ Carbon diffusion in the vicinity of a dislocation

200,000 KMC simulations = paths followed by 200,000 non-interacting carbon atoms.





Edge dislocation:

- C trapping (≈ 34% vs. 27%)

Screw dislocation:

- C trapping (≈ 32% vs. 27%)

R.G.A. Veiga, M. Perez, C.S. Becquart, E. Clouet & C. Domain, Acta Mater. 59 (2011) 6963.

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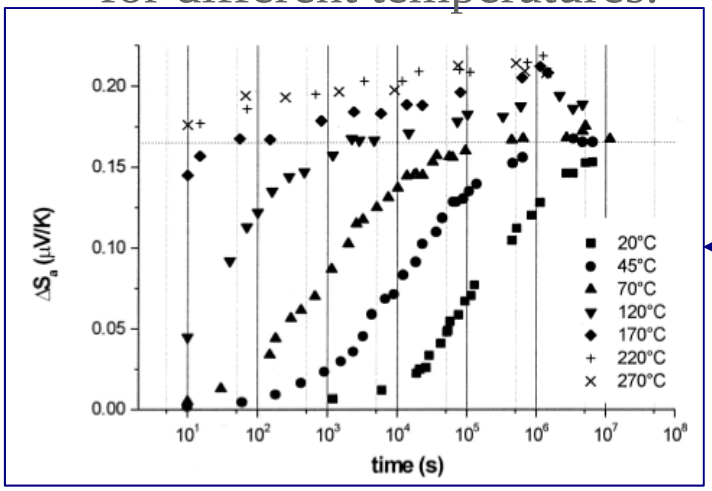
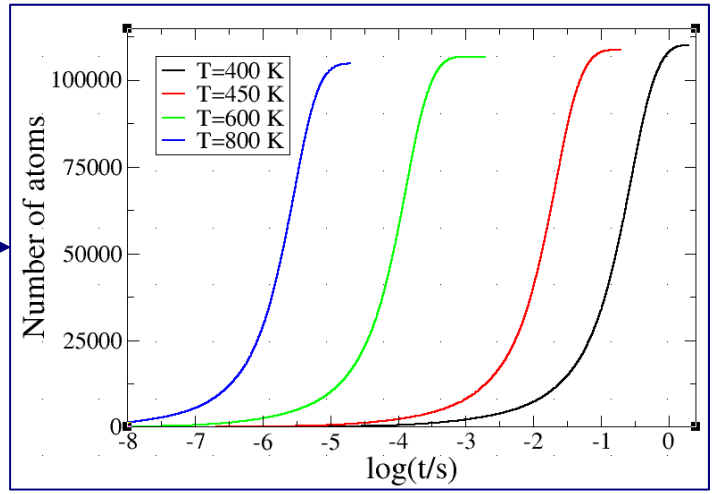
1/ Carbon diffusion in the vicinity of a dislocation

Figure 3. Strain ageing kinetics of ULC steel after cold rolling (50% of reduction) for different temperatures.



TEP measurements obtained from Lavaire et al.

Lavaire et al. Scripta mater. 44 (2001) 553.



Number of carbons arriving at an edge dislocation calculated by KMC.

TEP: Sensitive to carbon content in solid solution, but not in the dislocation, KMC results can be compared to TEP (in principle)

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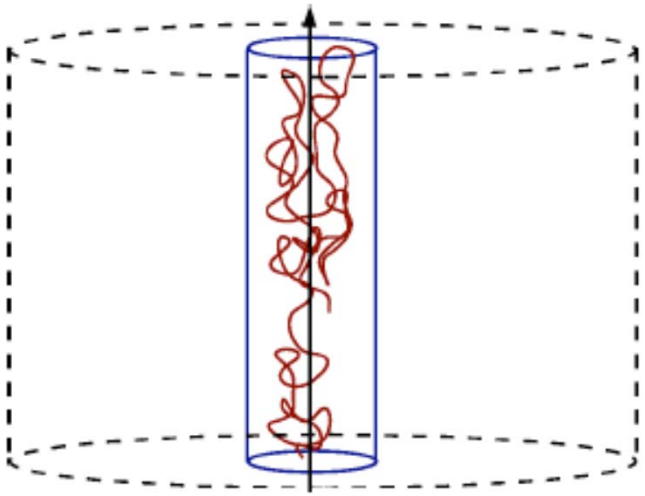
2/ Carbon diffusion in the core of a dislocation

(Quasi)-1D pipe diffusion



Within R < 1 nm: distorted lattice--> T-site as saddle point assumption no longer valid --> E_m calculated with the NEB

Large variation of E_m near the dislocation line

Lowest E_m :
0.14 eV (edge)
0.19 eV (screw)

Highest E_m :
1.55 eV (edge)
1.14 eV (screw)

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2/ Carbon diffusion in the core of a dislocation

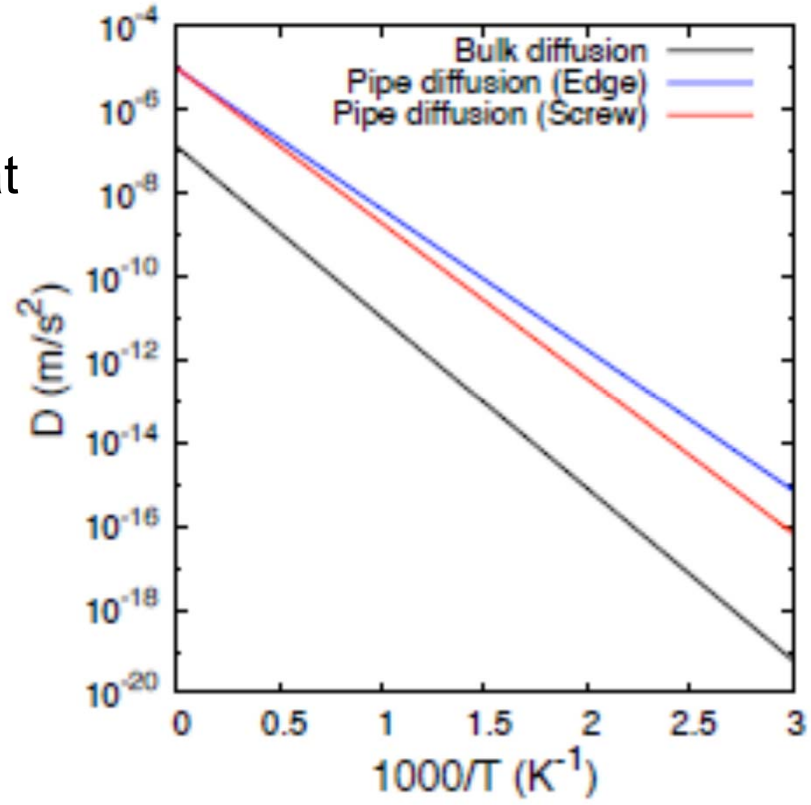
- < 400 K (edge) and < 750 K (screw)
  No diffusion is observed!
- ≥ 400 K (edge) and ≥ 750 K (screw)
  Some unidimensional (pipe) diffusion observed

From long trajectories (1,000,000 jumps) at high *T*:

Calculate $D = \langle [z(t)]^2 \rangle / 2t$

Activation energy --> slope log$D(1/T)$

0.67 eV (edge)
0.74 eV (screw)
0.82 eV in the bulk



Agreement with exp: enhanced diffusivity in the dislocation channel [Legros]

M. Legros, G. Dehm, E. Arzt and T. J. Balk. Science, 319, 2008, 1646.

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3/ Carbon distribution in a Cottrell atmosphere

Statistical model (Louat) based on the binding energies + MC

N. Louat. Proc. Phys. Soc. B, vol. 69, no. 459, 1956

Edge dislocation:

- Tension zone $\rightarrow E^b > 0$
- Compression zone $\rightarrow E^b < 0$
- Max $E^b = 0.65$ eV
- Min $E^b = -0.81$ eV

Screw dislocation:

- Three-fold rotational symmetry
- Max $E^b = 0.41$ eV
- Min $E^b = -0.58$ eV

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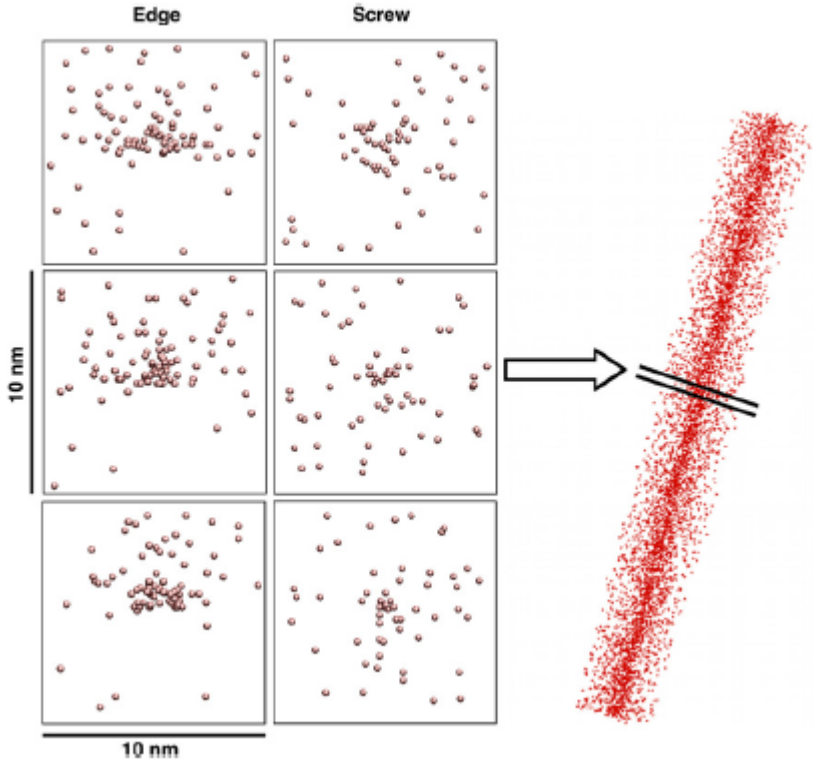
3/ Carbon distribution in a Cottrell atmosphere

Statistical model (Louat) based on the binding energies + MC

N. Louat. Proc. Phys. Soc. B, vol. 69, no. 459, 1956



Method	References	Dislocation	Extent (nm)	ϵ_{fac}
Atom probe	[Miller 2003, Miller 2006]	Unknown	10×10	7.7
Molecular statics	This work	Edge	15×6	6.3
	This work	Screw	8×8	5.4
Elasticity+DFT	[Hanlumyuang 2010]	Edge	20×20	5.3
	[Hanlumyuang 2010]	Screw	12×12	4.4

Roberto Veiga PhD thesis: september 2011: Computational insights into the strain aging phenomenon in bcc Fe at the atomic scale

1/ Carbon diffusion in the vicinity of dislocations: C atoms are attracted to dislocation cores

2/ Carbon diffusion in the core of a dislocation: confirmation of pipe diffusion

3/ Carbon distribution in a Cottrell atmosphere: enrichment factor in agreement with exp.

International Journal of Plasticity 62 (2014) 34–49

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International Journal of Plasticity

journal homepage: www.elsevier.com/locate/ijplas

Dislocation glide in Fe–carbon solid solution: From atomistic to continuum level description

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[a] Physics Department, Faculty of Science, Assiut University, Assiut 71516, Egypt
[b] EDF-R&D, MMC, Avenue des Renardières, 77818 Moret sur Loing, France
[c] SCK·CEN, Structural Materials Modelling and Microstructure Unit, SMA/NMS, Boeretang 200, 2400 Mol, Belgium
[d] Universitat Politècnica Catalunya, Jordi Girona 1-3, 08034 Barcelona, Spain

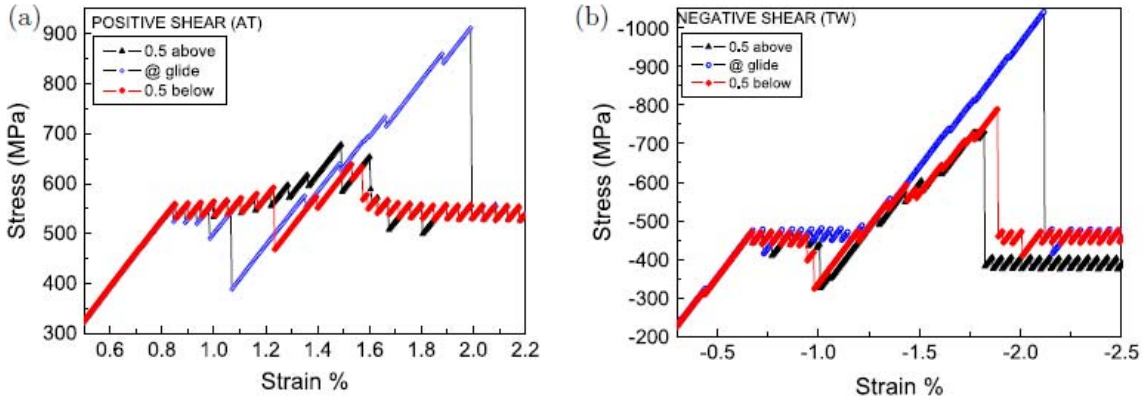

Fig. 7. Stress–strain curves for $1/2[1\,1\,1](1\,1\,\bar{2})$ edge dislocation overcoming a C atom at different positions. (a) Anti-twinning shear and (b) twinning shear.

-C solution: resistance of {112} slip plane lower than that of {110} plane.
-Complex collective effect of C atoms coupled with the residual lattice friction
==> weak softening effect could take place

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Scripta Materialia 108 (2015) 19–22

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journal homepage: www.elsevier.com/locate/scriptamat

Monte Carlo and molecular dynamics simulations of screw dislocation locking by Cottrell atmospheres in low carbon Fe–C alloys

R.G.A. Veiga [a,*], H. Goldenstein [a], M. Perez [b], C.S. Becquart [c]

[a] Escola Politécnica/Departamento de Engenharia Metalúrgica e de Materiais, Universidade de São Paulo, Av. Prof. Mello de Morais, 2463, Butantã CEP 05508-030, São Paulo/SP, Brazil
[b] Université de Lyon, INSA-Lyon, MATEIS, UMR CNRS 5510, 25 avenue Jean Capelle, F69621 Villeurbanne, France
[c] Unité Matériaux et Transformations (UMET), Ecole Nationale Supérieure de Chimie de Lille, UMR CNRS 8207, Bat. C6, F59655 Villeneuve d'Ascq Cedex, France

New model to build atmosphere: around a screw dislocation

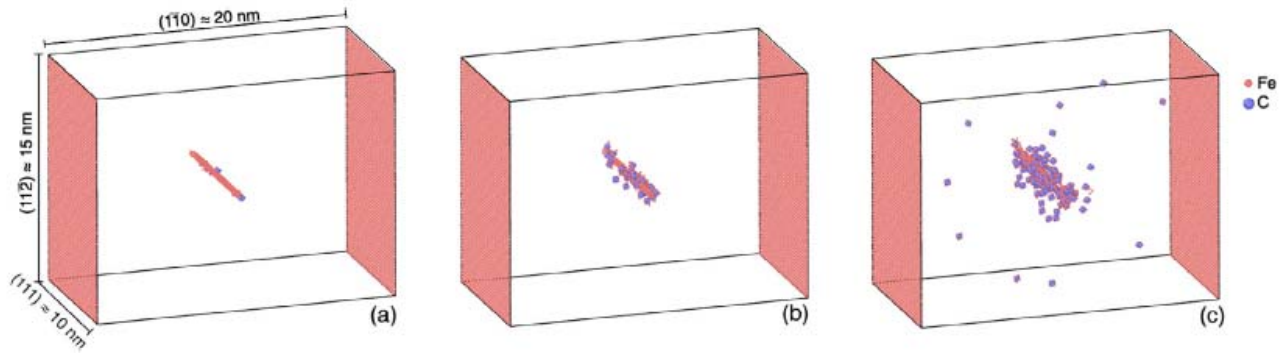

Fig. 1. MC-equilibrated carbon Cottrell atmospheres at $T = 300$ K for the systems with (a) 20, (c) 140 and (b) 500 ppm of carbon. Only non-bcc iron atoms (small red balls) and the carbon atoms (big blue balls) are shown for clarity. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

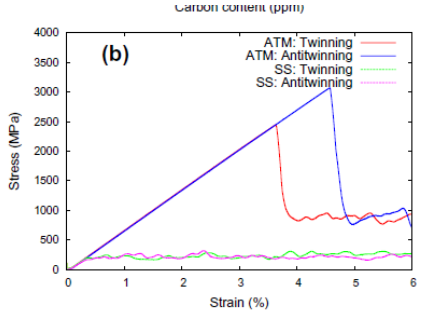

Fig. 3. (a) Stress required to unpin the screw dislocation from the Cottrell atmosphere as a function of carbon content. (b) Stress–strain curves associated with the systems containing 500 ppm of carbon: **ATM** is Cottrell atmosphere; **SS** is solid solution.

==> Very high unpinning stresses compared to C solid solution.

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Romain Candela PhD work (started december 2015)

Cottrell atmosphere formation at the atomic scale: k-ART. *Comparison with Metropolis MC and O. Waseda' PhD work.*

Dislocation – Cottrell atmosphere interactions at the atomic scale: *determination of the upinning stress (MD) at various temperatures and for atmospheres containing different levels of C or Mn (using existing FeC and FeMn potential), C and Mn (if a FeMnC potential is published).*

Cottrell atmosphere re-formation at the atomic scale: k-ART
Kinetic of C atoms rearrangement after the dislocation has moved away from the Cottrell atmosphere.

Cottrell atmosphere and dislocation motion at the mesoscale: phase field
Possibility to ***study collective dislocation interactions.***

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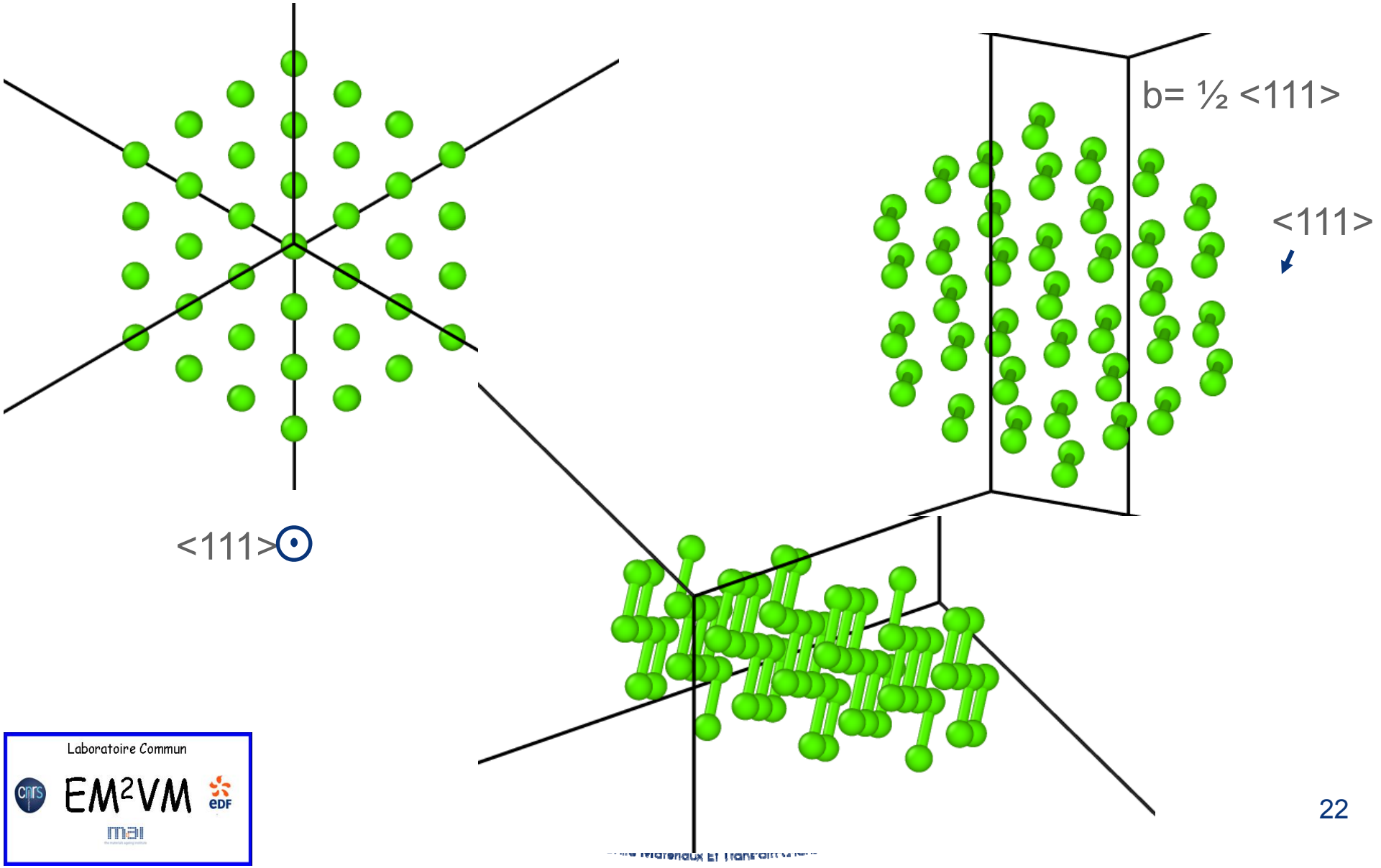
I37 <111> loop



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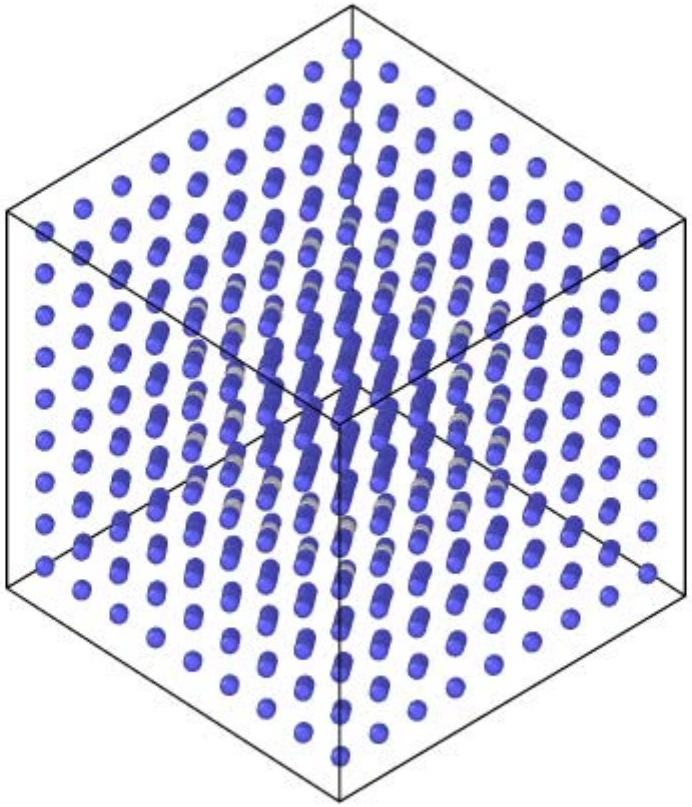
I37 <111> loop: structure

- bcc
- other

Common neighbour analysis OVITO



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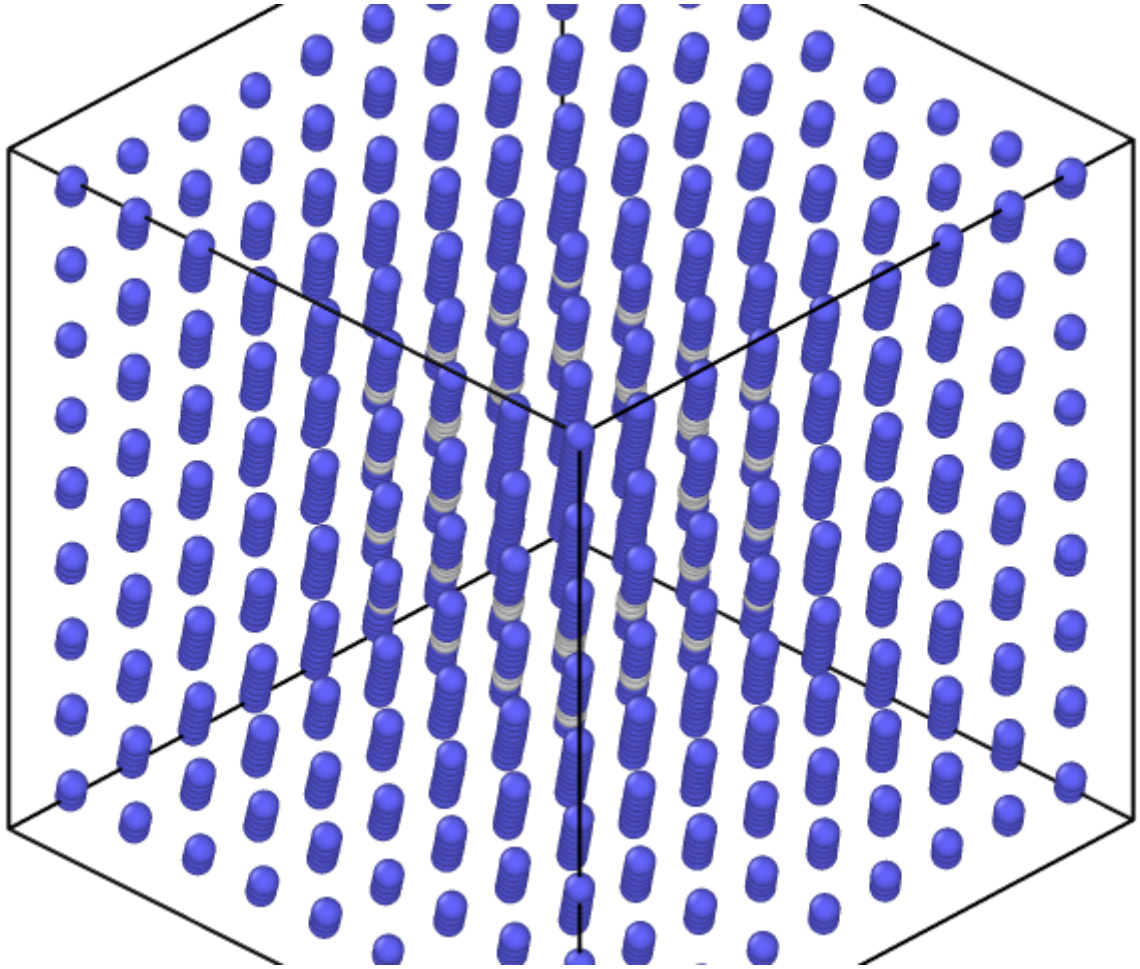
I19 <111> loop: structure

Common neighbour analysis OVITO

bcc

other



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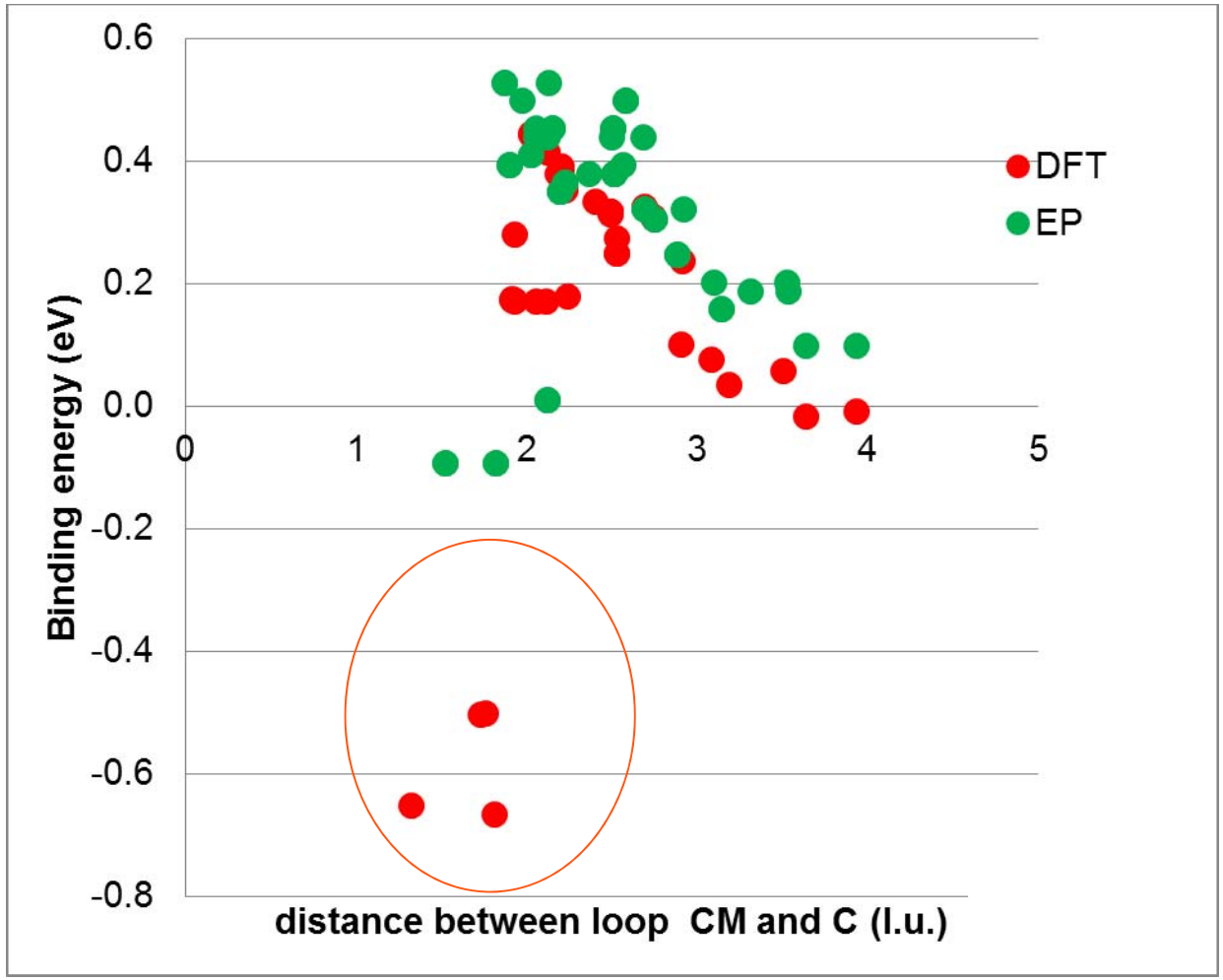
The **torus geometry is valid** for quite small loop sizes

C- I19 loop binding energy



DFT and EP relax differently

Distances similar: the **relaxation with EP not very large most of the time.**

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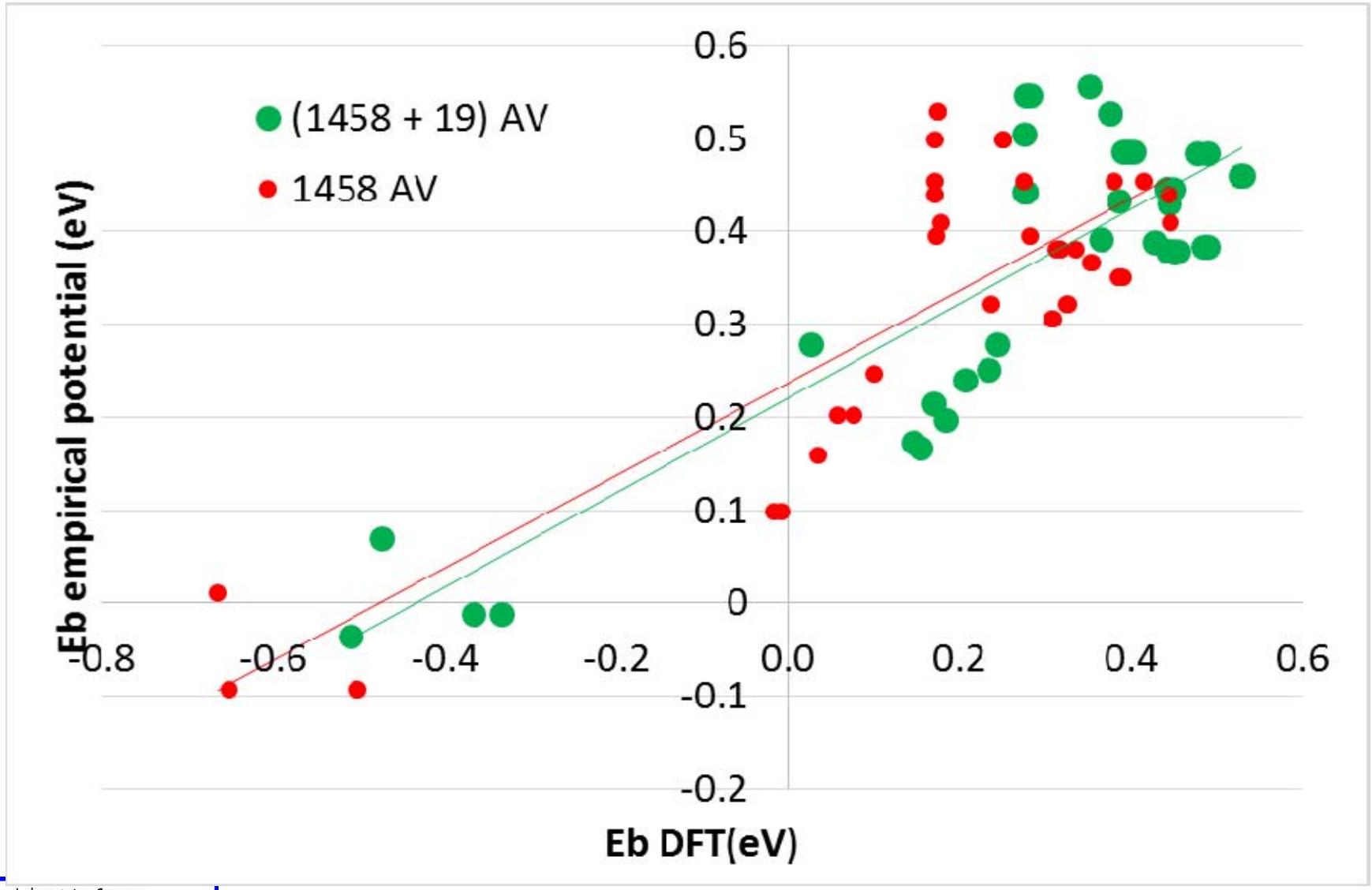
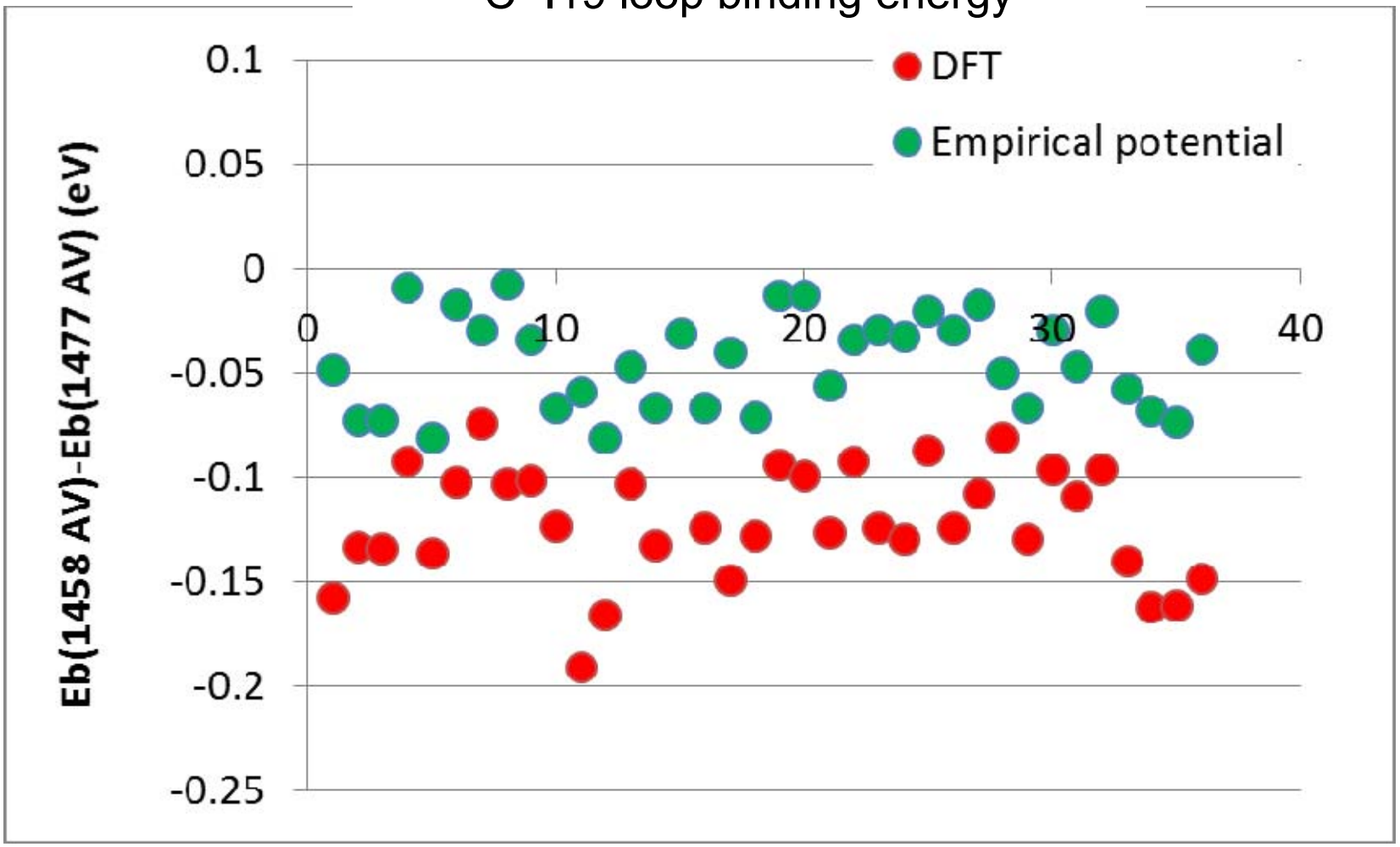
C- I19 loop binding energy



C- I19 loop binding energy



DFT more sensitive to box volume

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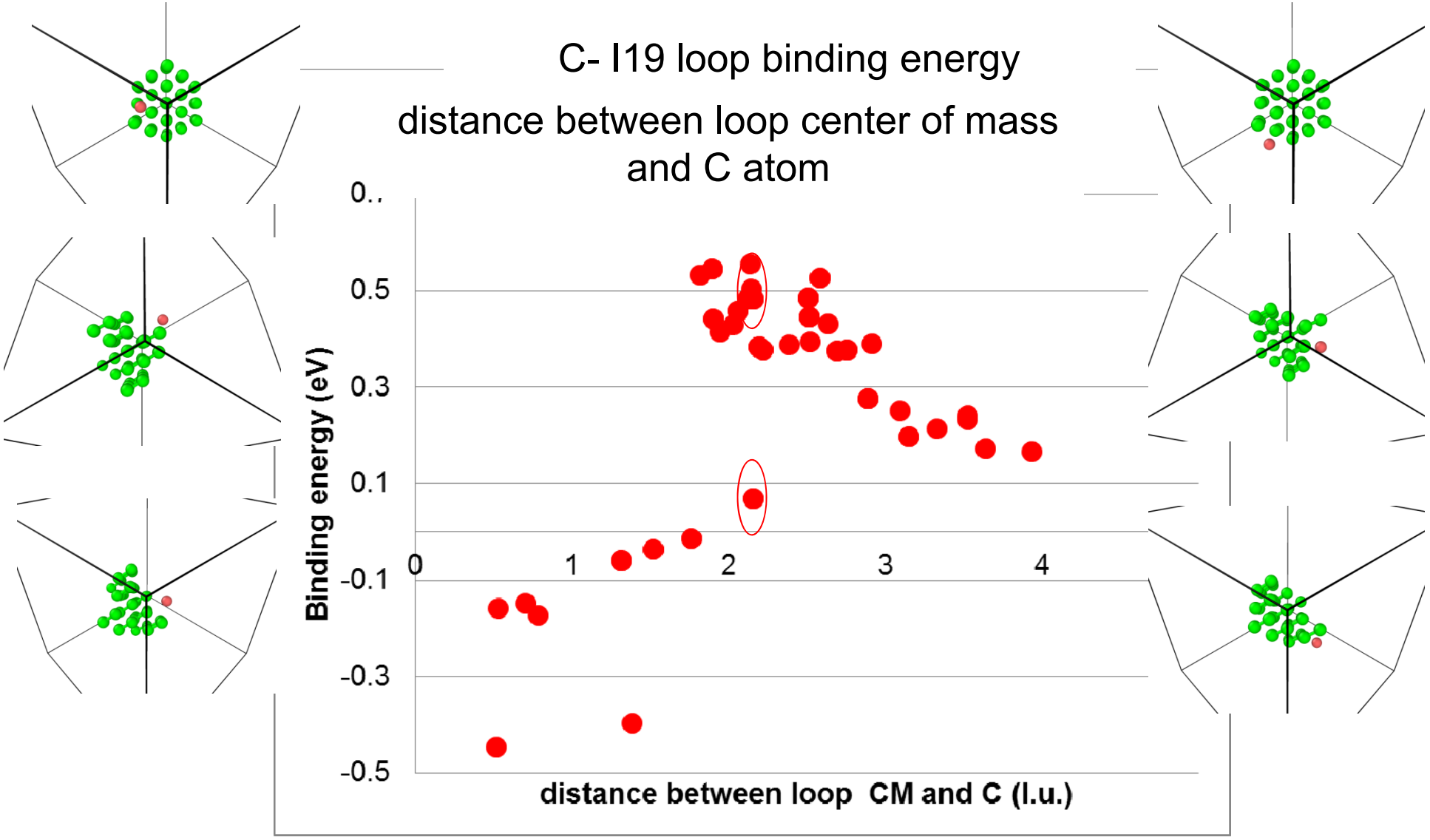
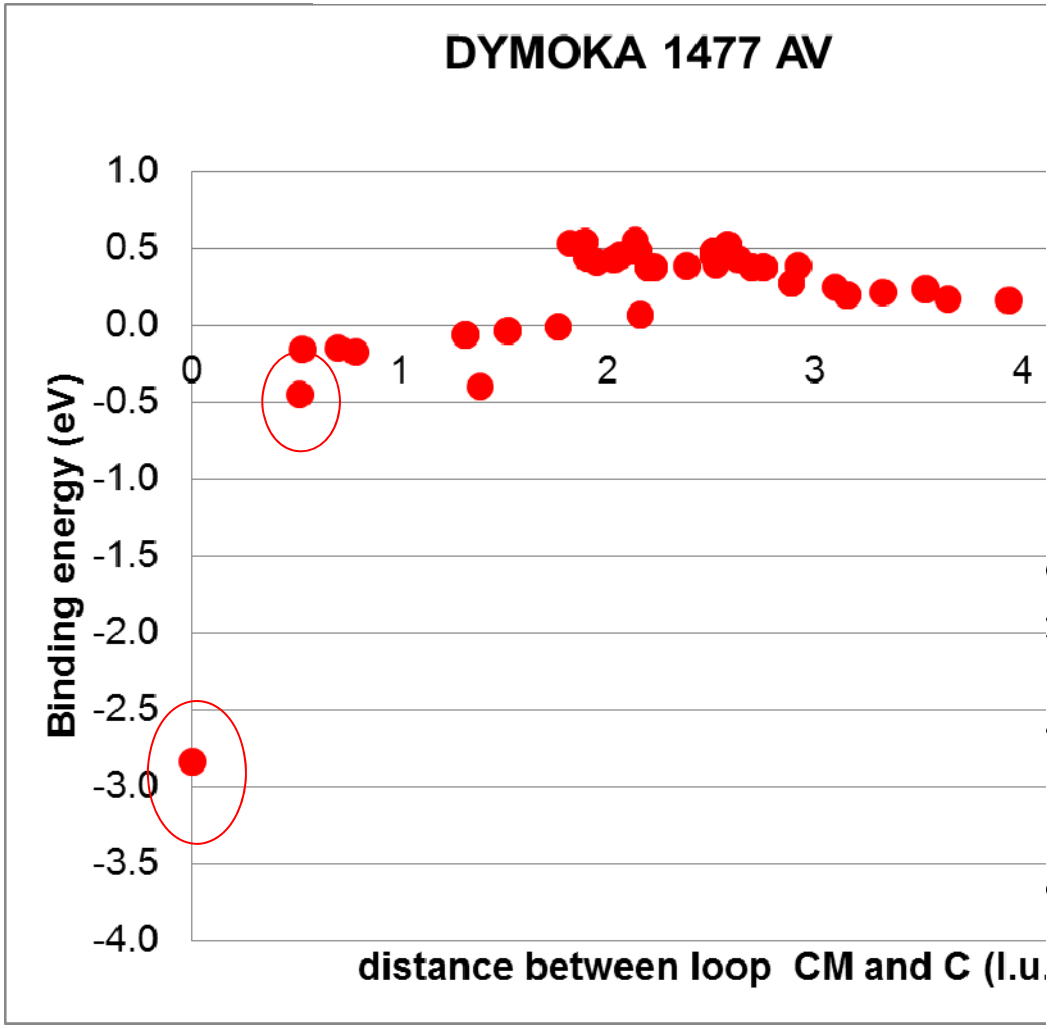
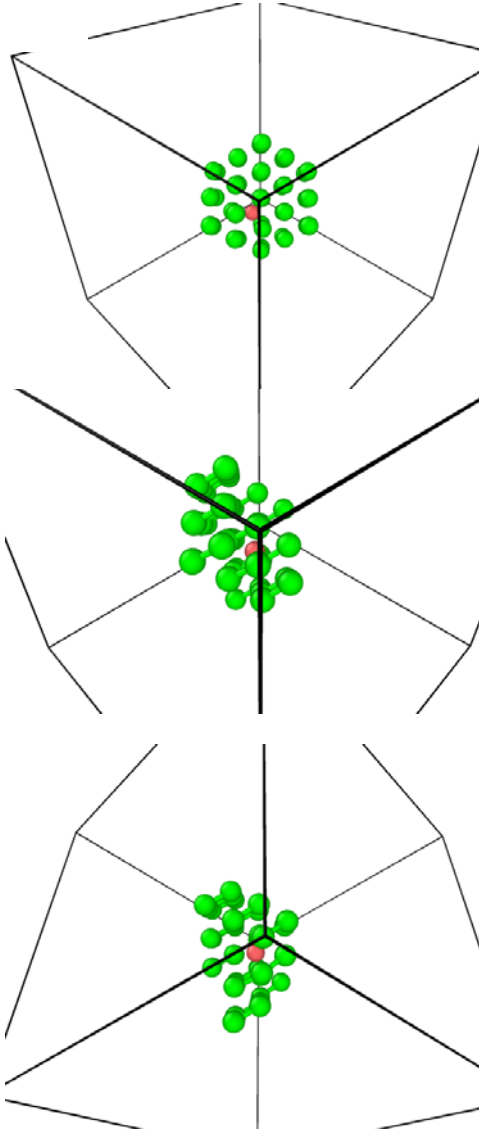


EP + box + 19 atomic volumes

C- I19 loop binding energy





EP + box + 19 atomic volumes

Repulsion inside the loop

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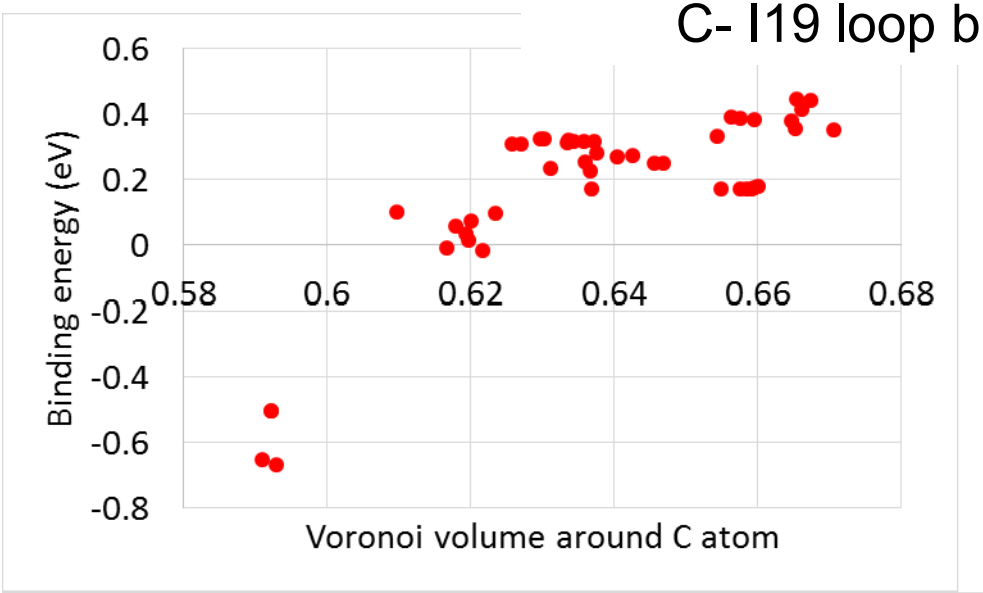
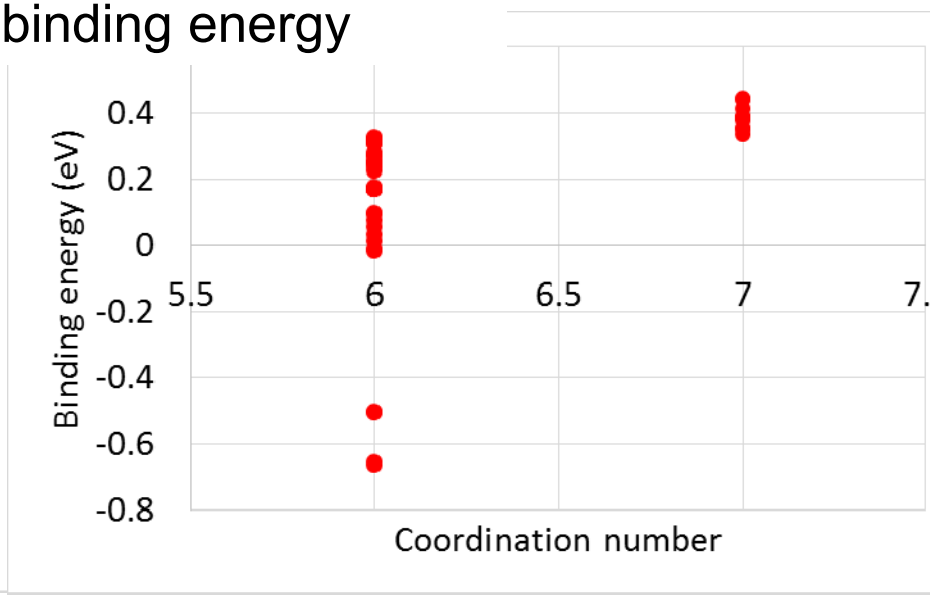
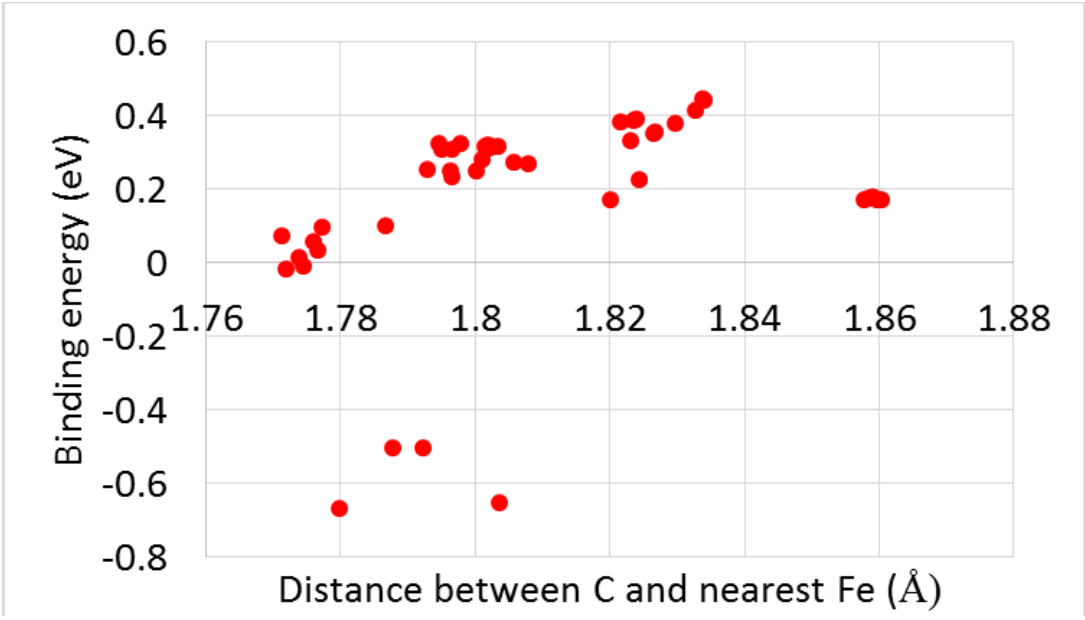
C- I19 loop binding energy



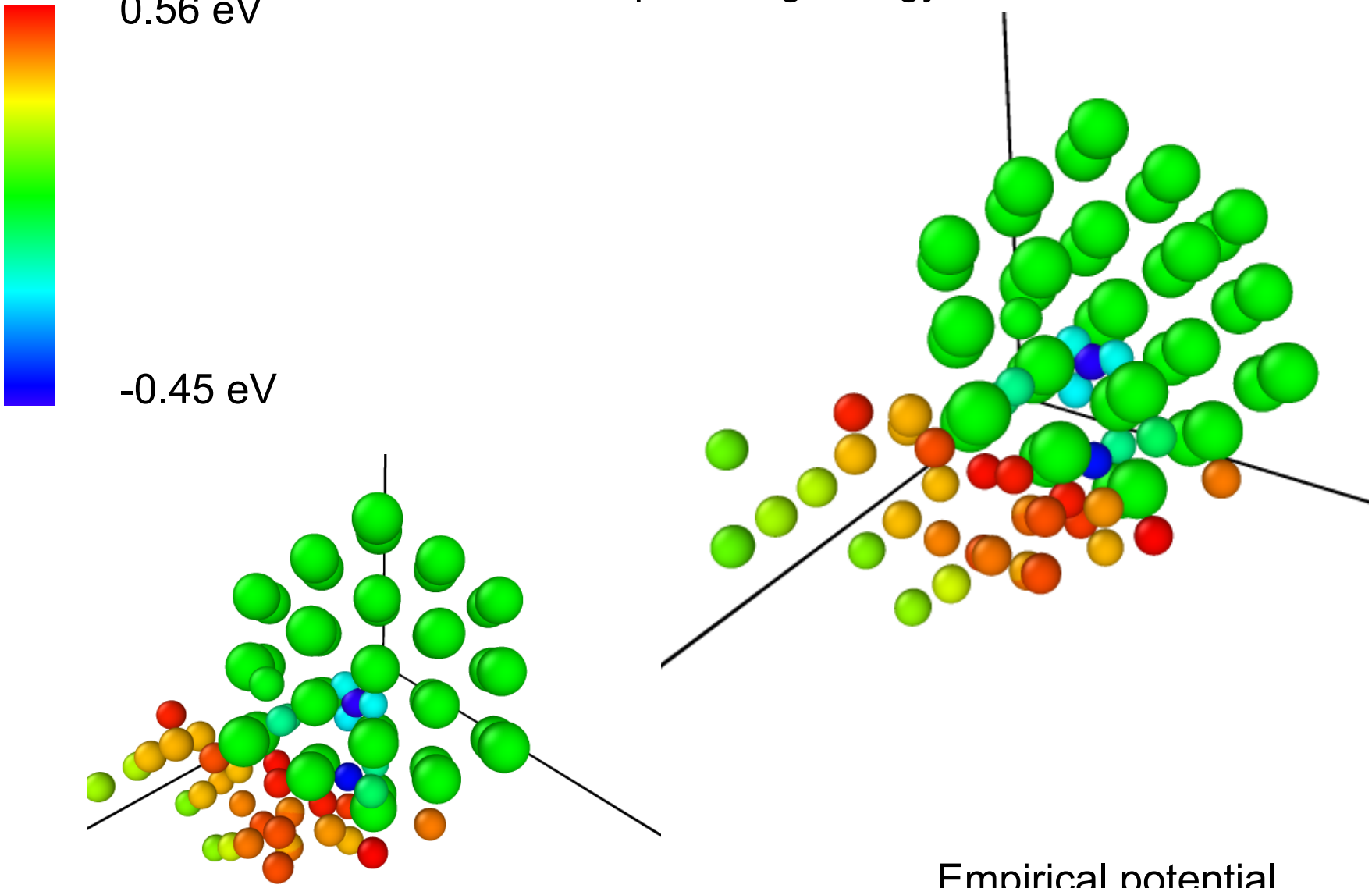


DFT, 1458 AV



-The highest binding energy sites have the highest coordination number
-Good trends with the Voronoi volume

C- I19 loop binding energy



Empirical potential

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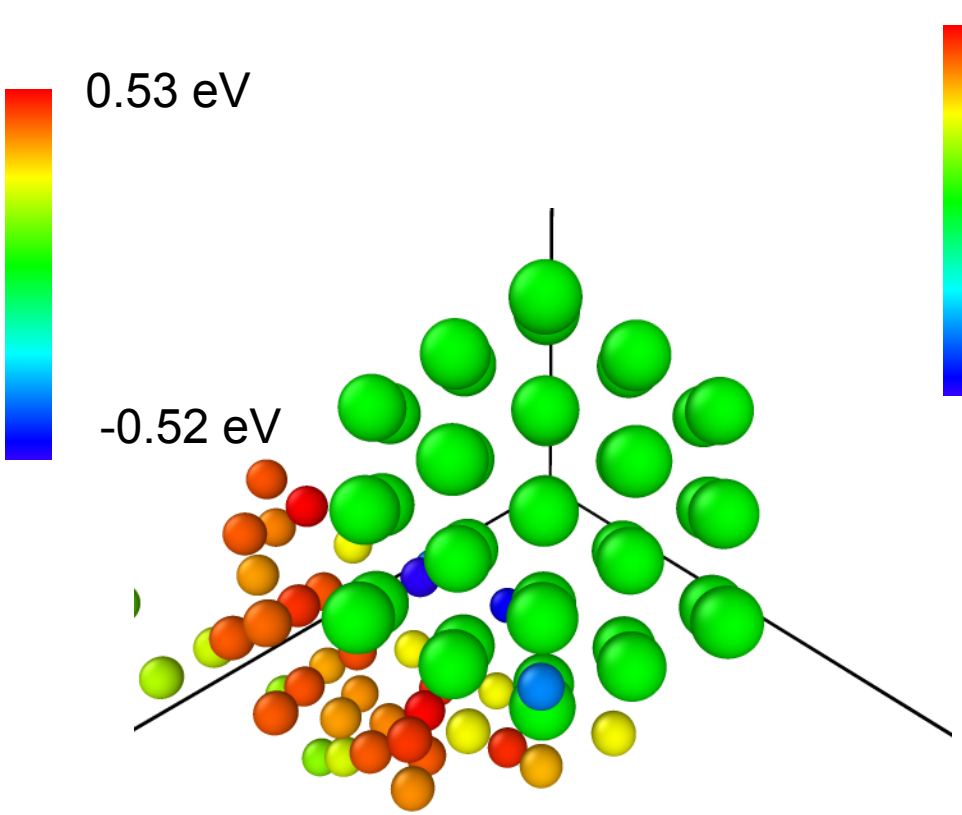
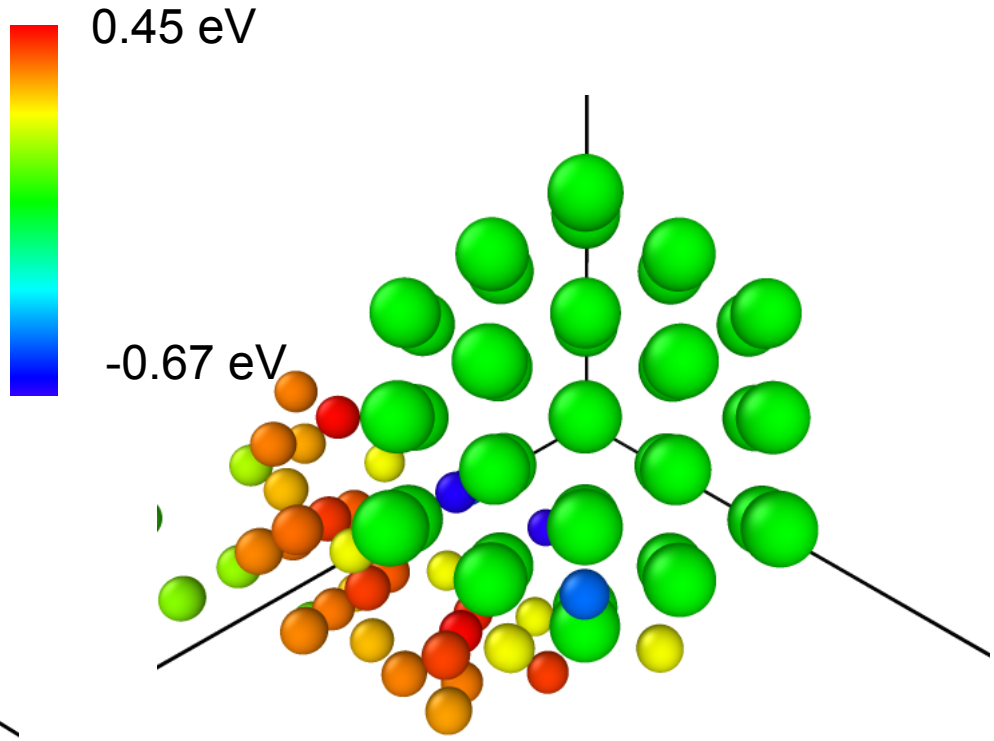
C- I19 loop binding energy



DFT: 1458 AV



DFT: 1477 AV

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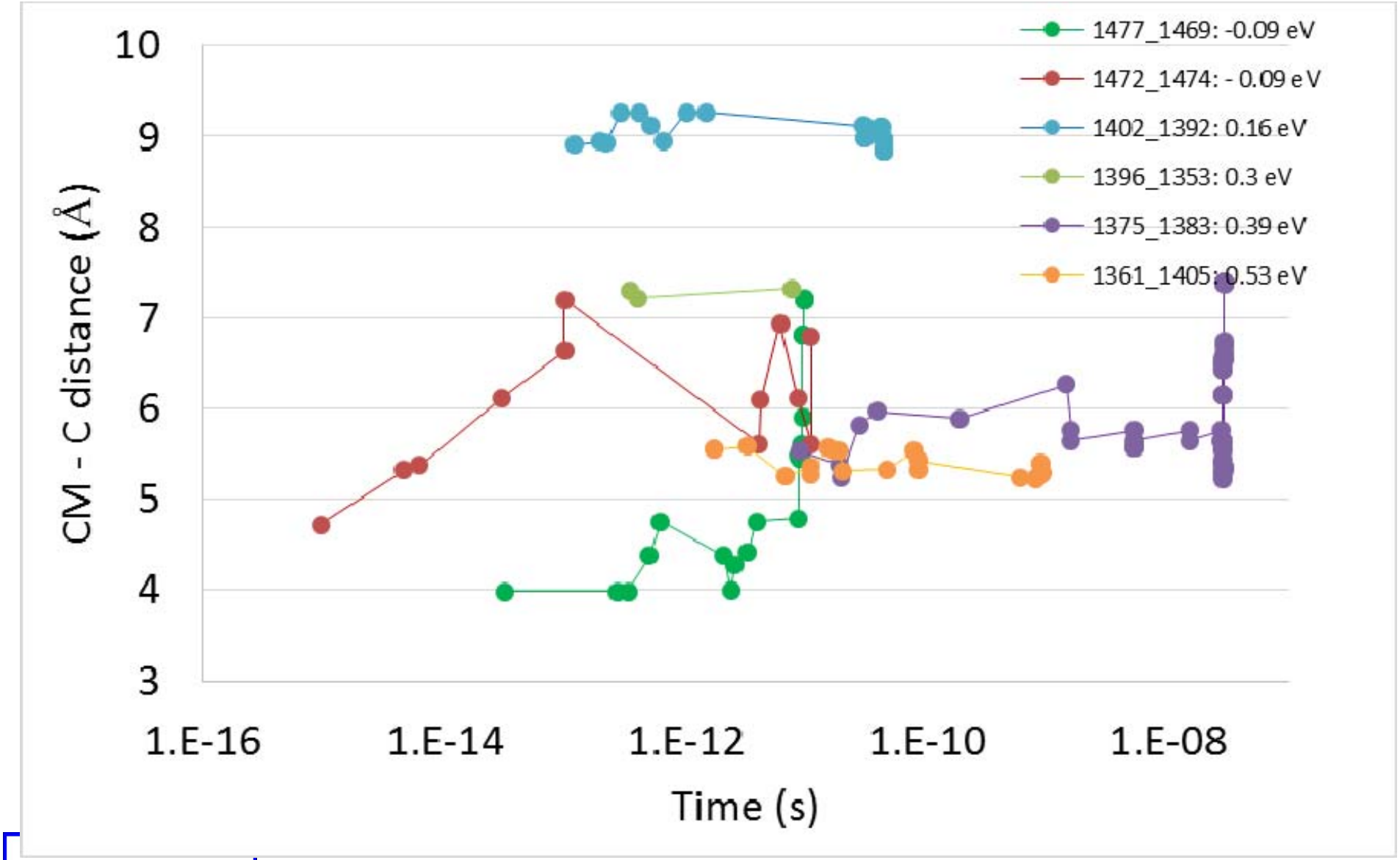
K-ART

Special thanks to
Calcul Québec
Calcul Canada

-300 K
-1478 atoms: 19 SIA <111> loop + 1 C atom
-300 K lattice parameter + 19 atomic volumes

-12 processors

K-ART simulations at 300 K



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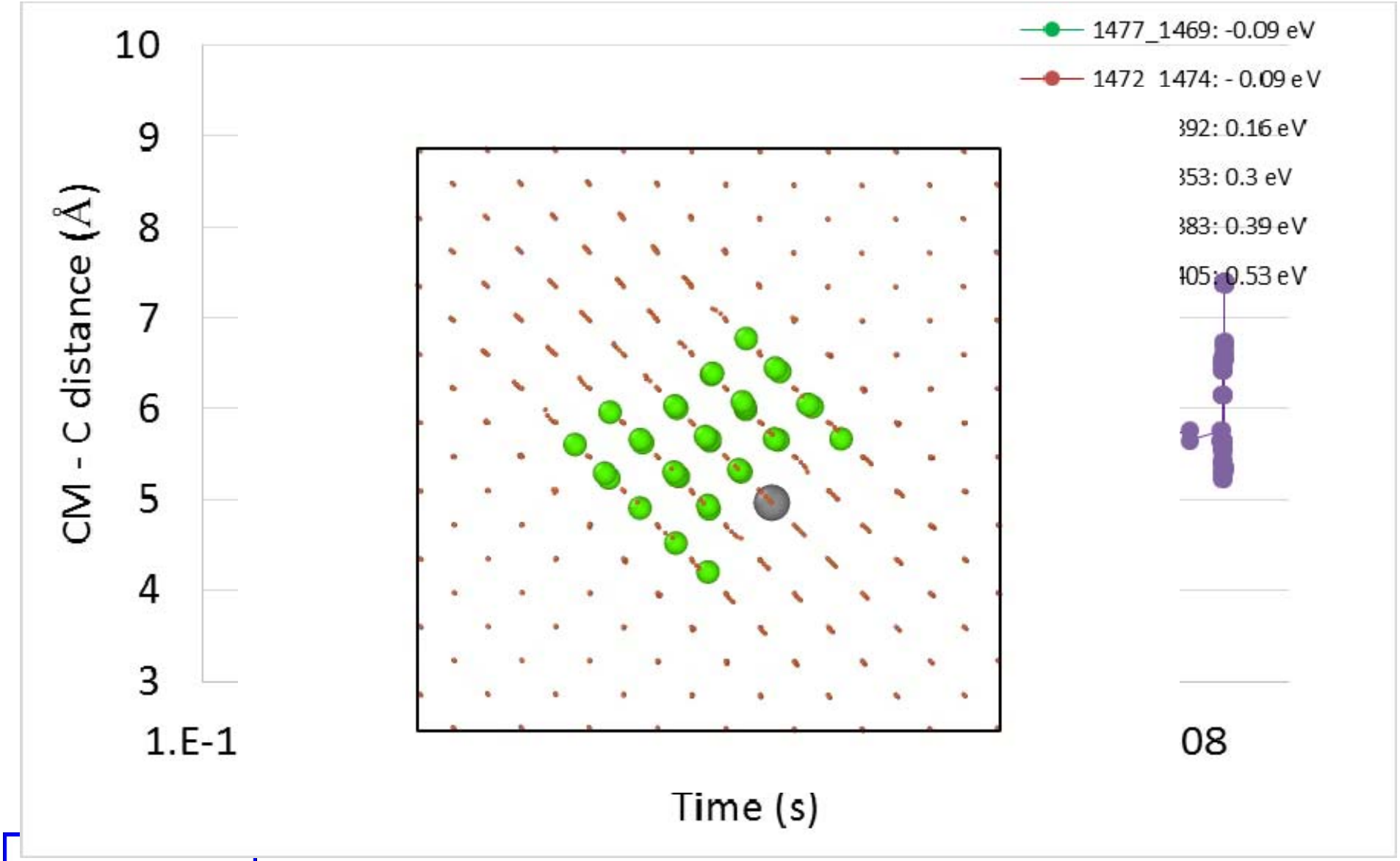
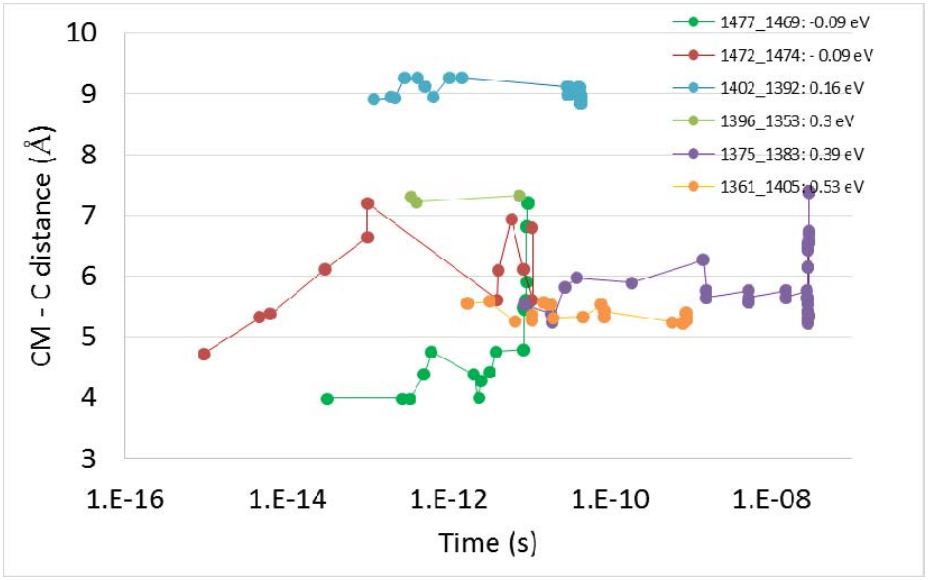
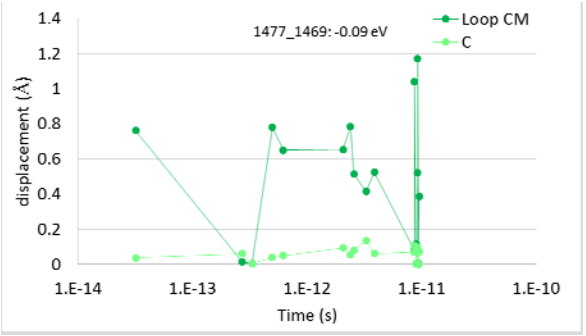
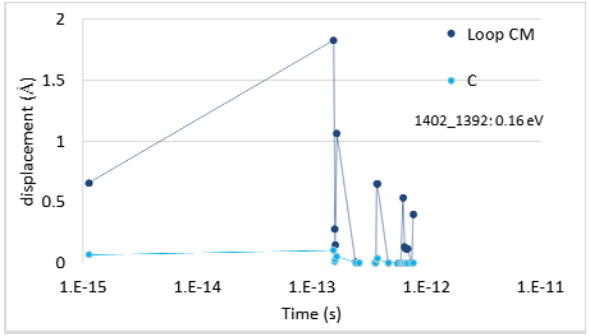
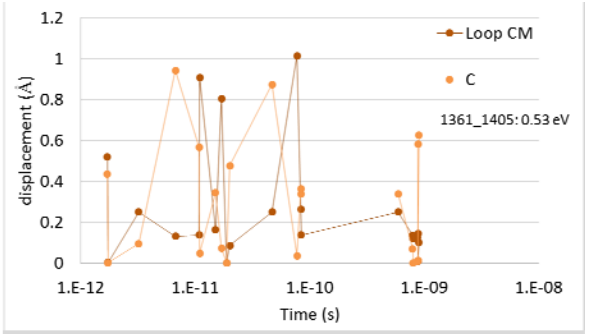
K-ART simulations at 300 K











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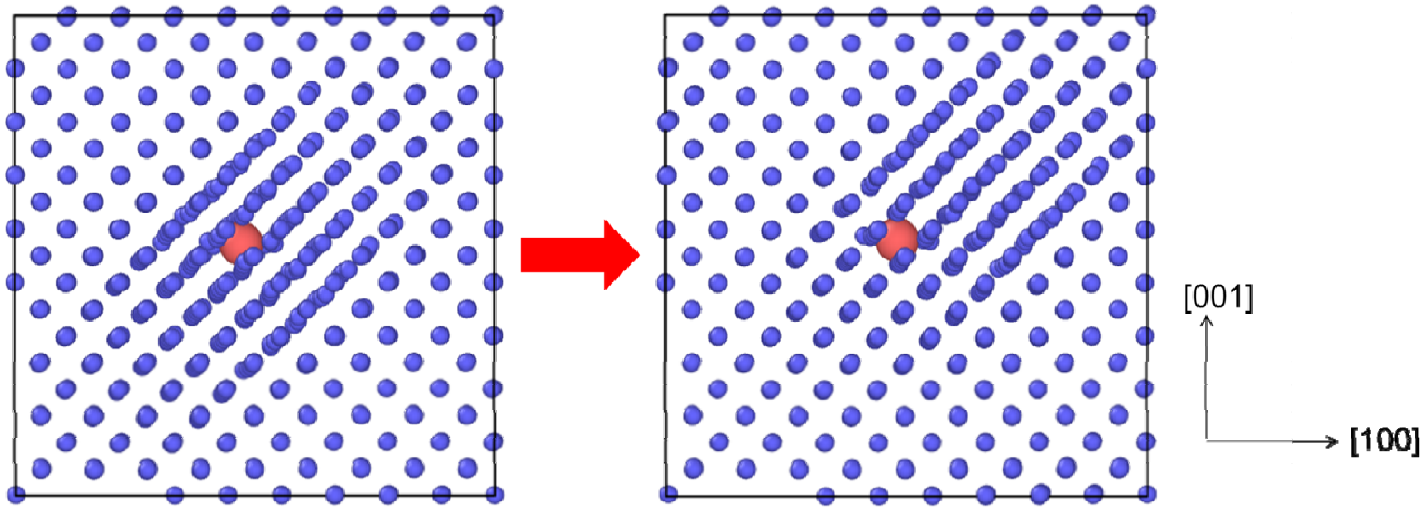
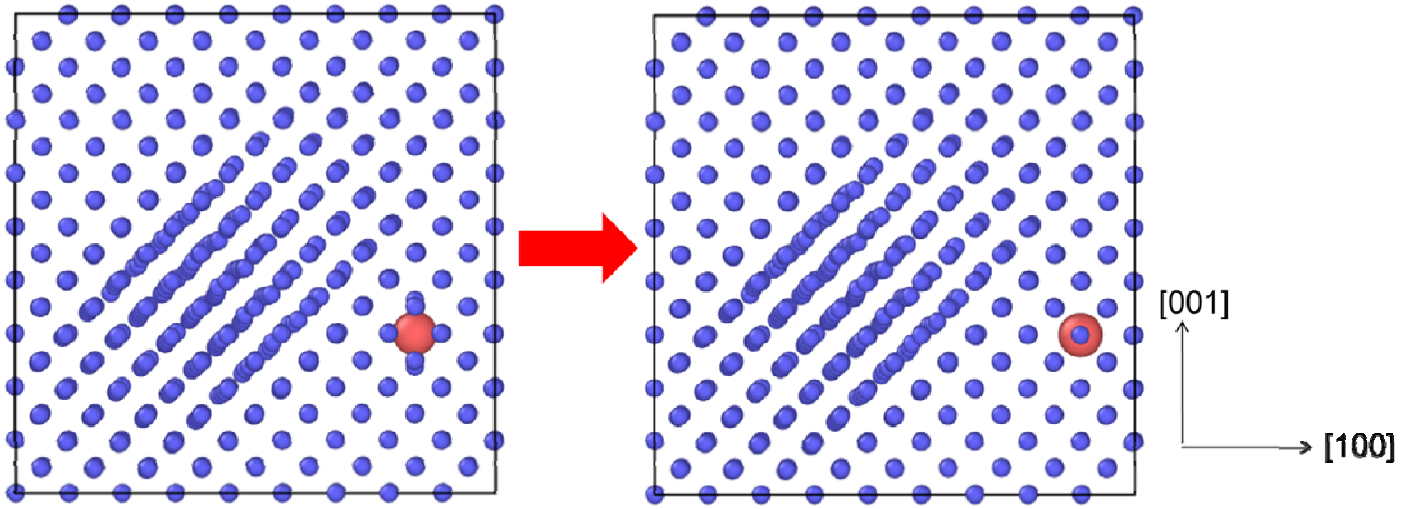
Method 1: the C atom (red atom) is placed near the Fe (blue atoms) loop



t = 0 s

t = $3.323.10^{-13}$ s

Method 2: all the transitions with an energy < 0.2 eV are ignored ➔ only the C will move



t = 0 s

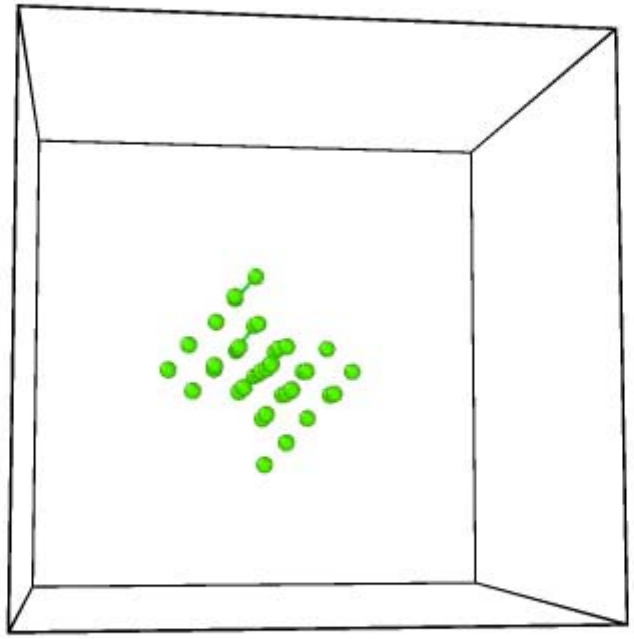
t = $3.930.10^{-9}$ s

Average time step for a C jump: ~ 8.10^{-8} s
Average time step for a loop displacement: ~ 8.10^{-15} s.

The loop moves way faster than the C atom ==> the loop needs to be pinned for the atmosphere to form.

Average time step for a C jump: ~ 8.10^{-8} s
Average

The loo ds to
be pinn



MD: 300 K.
Dt = 3 10^{-15} s
Total time: 1.5 ns
Box = 11 x 11 x 11 u.c.

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Perspectives

-On going work

-Pin the loop with many C atoms

-Couple k-ART with regular AKMC with Lincos approach