



POLITÉCNICA



Universitat d'Alacant  
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# *MMonCa: A flexible and powerful new Kinetic Monte Carlo Simulator*

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[www.materials.imdea.org](http://www.materials.imdea.org)

# Outline

- Why new code?
- The KMC algorithm & Object KMC: Rates
- MMonCa:
  - Ideas
  - Implementation
  - Physical mechanisms
  - Flexibility
- Examples
  - Isochronal annealing of a-Fe
  - Annealing of implanted defects in Si
  - Evolution of damage in W
- Conclusions

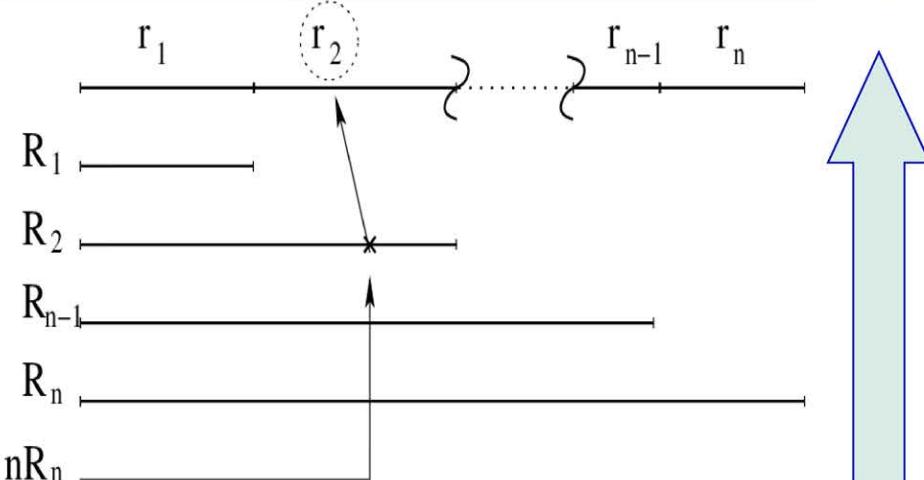


# Why developing new code?

- Kinetic models must reach high irradiation doses for very complex systems
  - Point defects and impurities
  - Extended defects, dislocations
  - Clusters (with helium, carbon...)
- So far there are no easy available “standard” KMC simulators.
- There is a need for **efficiency** and **flexibility**.

# The KMC algorithm

- determine all possible processes for a given configuration and build a list of their rates  $r_i$  (e.g. I jump, V jump, I emission from defect)



calculate the total rate of events  $R=\sum r_i$

generate a random number  $n \in [0,1)$

use  $n$  to select an event from the list  
(e.g. "This Interstitial will jump")

Perform the event. Manage interactions between particles.

Advance time. New time = old time +  $1/R$

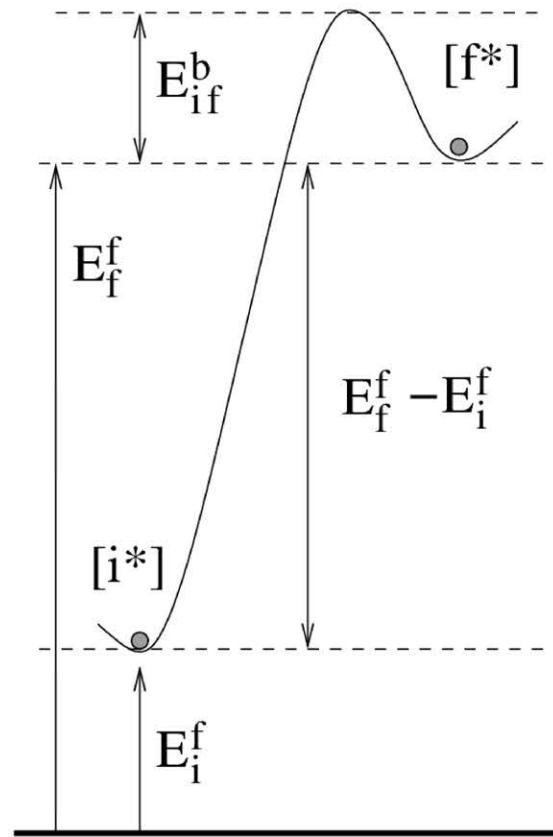
End

# Object KMC: Rates

- All different rates are assumed to be produced by a **prefactor** and an activation energy
- The **activation** energy is computed as the difference in formation energies between final and initial states plus a barrier (typically a migration energy)

$$E_{ij} = E_j^f - E_i^f + E_{ij}^b$$

$$r_{ij} = P_{ij} \times \exp(-E_{ij}/k_B T)$$

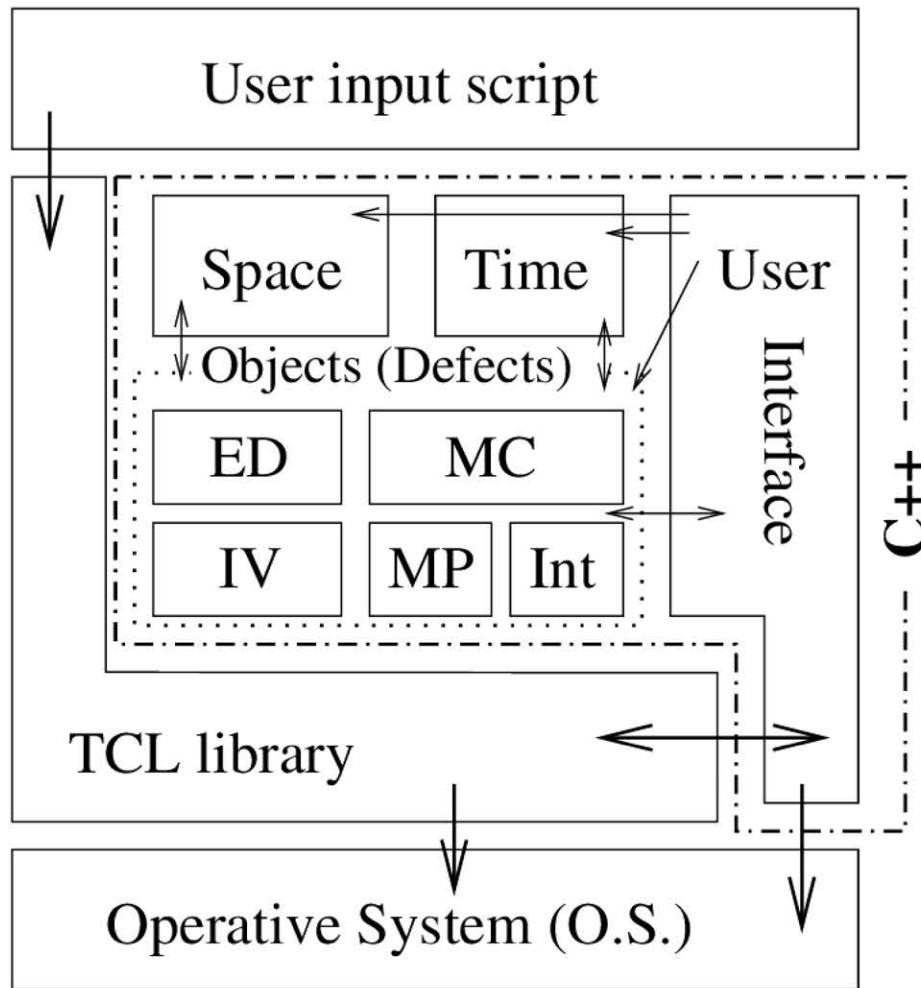


# Development ideas

- **Modular**: Possibility for Object KMC, Lattice KMC and maybe others.
- **Versatile** and **flexible**: Build on top of Tcl scripting language.
- **Efficient** and **modern**: Written using Object Oriented Methodologies in C++
- **Professional** development, debugging, profiling and testing
- **User oriented**: Customizable through input files rather than code changes.



# MMonCa: Implementation



- Four main areas: **space**, **time**, **user interfaces** and **defects**
- Defects belong to 5 categories: **Extended Defects (ED)**, **Mobile Particles (MP)**, **Multi Clusters (MC)**, **IV Damage (IV)** and **Interfaces (Int)**.

# OKMC mechanisms

- Diffusion
  - I, V, C, He, ...
  - $\text{He}_nV_m$ , ...
  - $I_n, V_m$ , ...
- Cluster emission
  - $\text{He}_nV_m \leftrightarrow \text{He}_{n-1}V_{m-1} + \text{HeV}$
  - $\text{He}_nV_m \leftrightarrow \text{He}_{n-1}V_m + \text{He}$
  - $\text{He}_nV_m \leftrightarrow \text{He}_nV_{m-1} + V$
  - $\text{He}_nV_m \leftrightarrow \text{He}_{n-1}V_{m+1} + I$
- Very complex clusters
  - $\text{He}_nC_mV_o \leftrightarrow \text{He}_nC_{m-1}V_o + C$
  - ...
- Extended defects
  - $I_n \leftrightarrow I_{n-1} + I$
  - $I_n(A) \leftrightarrow I_n(B)$
  - $I_n + \text{Trap (mobile)} \leftrightarrow I_n \text{ Trapped (immobile)}$
- Damage
  - $I_nV_m \rightarrow I_{n-1}V_{m-1}$
- Interfaces
  - $\text{MPA} + A/B \leftrightarrow \text{MP}(A/B) \leftrightarrow \text{MPB} + A/B$
  - $\text{MP} + A/B \leftrightarrow A/B$
  - $\text{ED} + A/B \leftrightarrow A/B$
  - $\text{MC} + A/B \leftrightarrow A/B$
  - $\text{Int} \rightarrow \text{Int} + I$

# Flexibility in MMonCa

- IDEA: The **tcl** language is used to allow **flexibility**.
- User defined:
  - The material **structure** (full 3D)
  - All the clusters and extended defect **rates**
  - Reactions, using **wildcards**
- Default parameters can be overwritten in the **input** file: **self-contained**

```
array<string,string> interactions {  
    He*+Hei true  
    He*+V  true  
    He*+Gas true  
    C*I*+I true  
    C*V*+V true  
}  
  
proc migrate { size } {  
    if { $size == 2 } { return "8.2e-3 0.42" }  
    if { $size == 3 } { return "8.2e-3 0.43" }  
    if { $size == 4 } { return "8.2e-3 0.43" }  
    set pref [expr 3.5e-4+1.7e-3/pow($size,1.7)]  
    set ener [expr 0.06+ 0.11/pow($size,1.6)]  
    return "$pref $ener"  
}  
  
proc material { x y z } {  
    if { $x < 0 } { return "Copper" }  
    return "Niobium"  
}
```



Group → Period ↓

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																2 He	
2	3 Li	4 Be															10 Ne	
3	11 Na	12 Mg															18 Ar	
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co		29	30	31	32	33	34	35	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh		47 Ag	48 Cd	49 In	50 Ge	51 Sn	52 Sb	53 Te	54 Xe
6	55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir		79 Au	80 Hg	81 Tl	82 Pb	83 Po	84 At	85 Rn	
7	87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo

Lanthanides

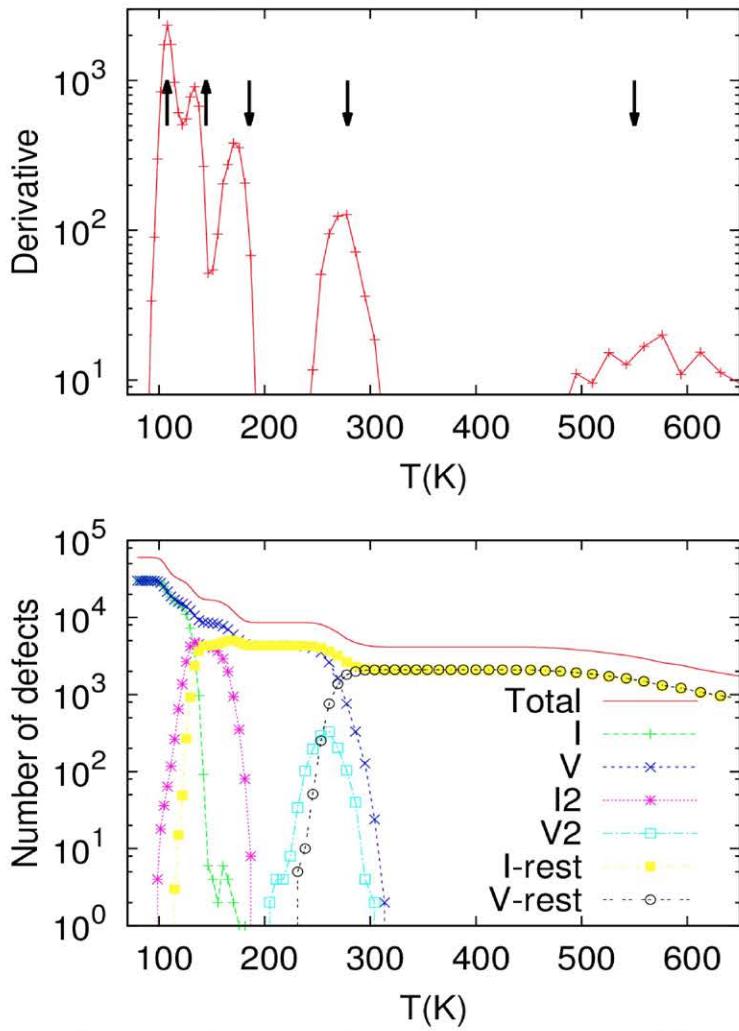
57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Actinides

# Isochronal annealing of $\alpha$ -Fe



# Defects and resistivity recovery during $\alpha$ -Fe annealing



- Simulated isochronal annealing of  $2e-4$  dpa irradiated Fe.
- Excellent agreement with experiments<sup>1</sup> and simulations.<sup>2,3</sup>

<sup>1</sup> Takaki et al. Radiation Effects 79, 87 (1983)

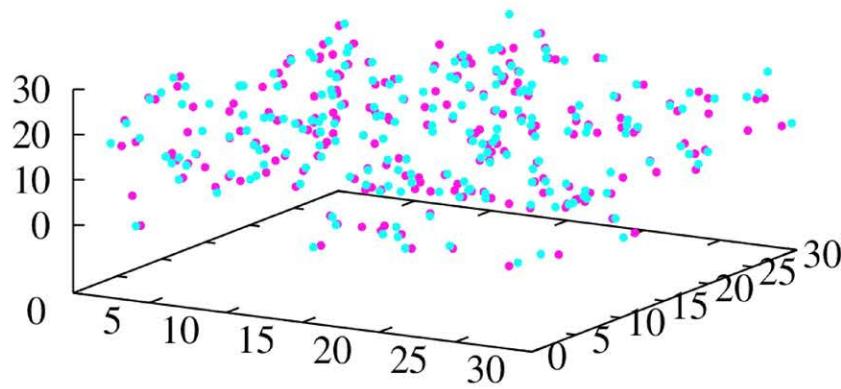
<sup>2</sup> Fu et al. Nature materials 4, 68 (2005)

<sup>3</sup> Ortiz and Caturla. Phys. Rev. B 75, 1884101 (2007)

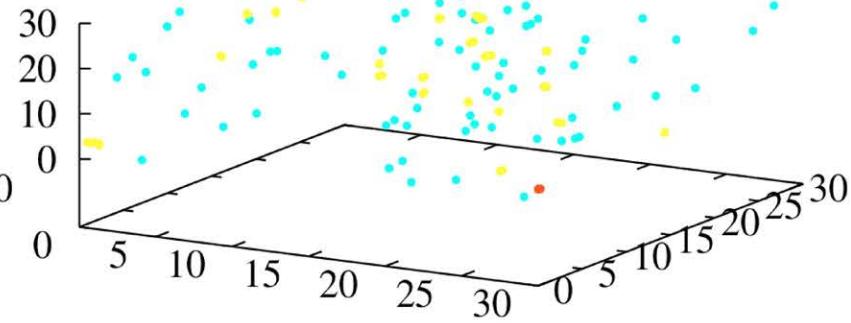


# Defect population evolution during annealing of $\alpha$ -Fe

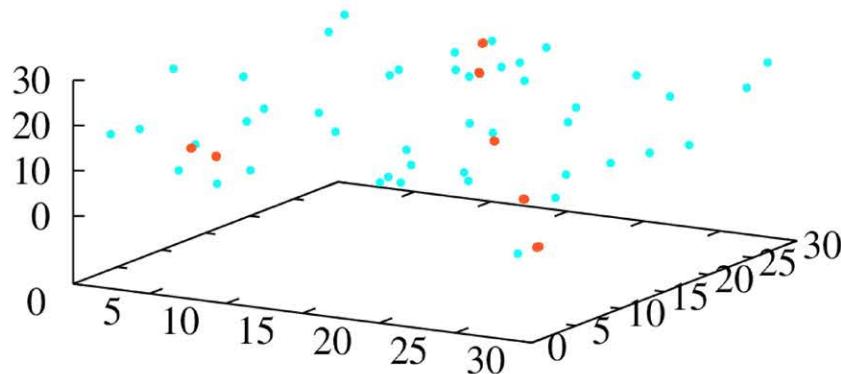
a) 107 K



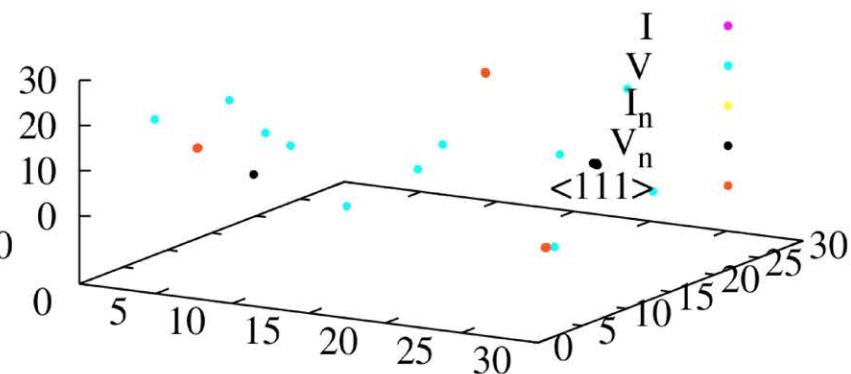
b) 146 K



c) 186 K



d) 277 K





Group → 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18  
↓ Period

1	H																2 He	
2	Li	Be															10 Ne	
3	Na	Mg															18 Ar	
4	K	Ca	Sc	T	V	Cr	Mn	F	Co	Ni	Cu	Zn	Ga	Ge	P	S	36 Kr	
5	Rb	Sr	Y	Zr	Nb	Mo	43	44	45	46	47	48	49	50	51	52	54 Xe	
6	Cs	Ba		72	73	74	W	75	77	78	79	80	81	82	83	85 At	86 Rn	
7	Fr	Ra		104	Rf	Db	Sg	107	Bh	109	Mt	110	Ds	111	Rg	112	117 Uus	118 Uuo

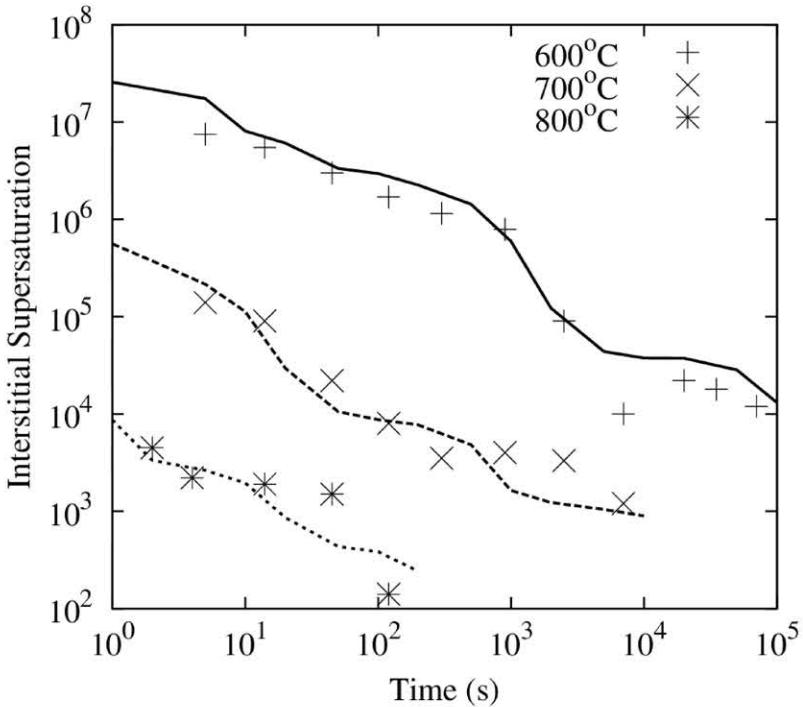
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Actinides

# Annealing of implanted defects in silicon

# Interstitial evolution in damaged Si



- Interstitial supersaturation  $[I]/[I^*]$  after a 40 keV,  $2e13$  cm-2 Si into Si implant annealed at different temperatures.
- Excellent agreement with experimental<sup>1</sup> results and previous simulations.<sup>2</sup>

<sup>1</sup> Cowern et al. Phys. Rev. Lett. 82, 4460 (1999)

<sup>2</sup> Martin-Bragado et al. Solid-State Electronics 52, 1430 (2008)



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# Evolution of damage in tungsten



	Particles	Clusters
Mobile	He V I	$\text{He}_n$ $\text{V}_n$ $\text{I}_n$
Immobile	C (as traps for V, I)	$\text{He}_n \text{V}_m$ $\text{He}_n \text{I}_n$ $\text{C}\text{V}_n, \text{C}\text{I}_n$

	$\text{He}_3$
Epot	-2.39 eV
Emission pref. ( $\text{He}_3 \rightarrow \text{He}_2 + \text{He}$ )	9.9856e-4 cm <sup>2</sup> s <sup>-1</sup>
Emig	0.05 eV
Migration pref.	9.9856e-6 cm <sup>2</sup> s <sup>-1</sup>

# MMonCa parametrization<sup>1</sup>

- Clusters defined by:
  - Potential energy
  - Emission prefactor
  - Migration prefactor
  - Migration energy
- The particle-cluster binding energy is calculated by MmonCa

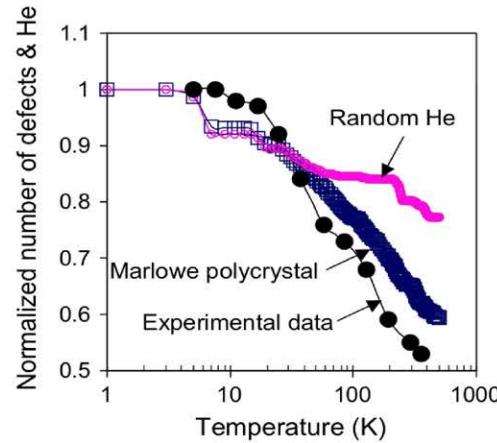
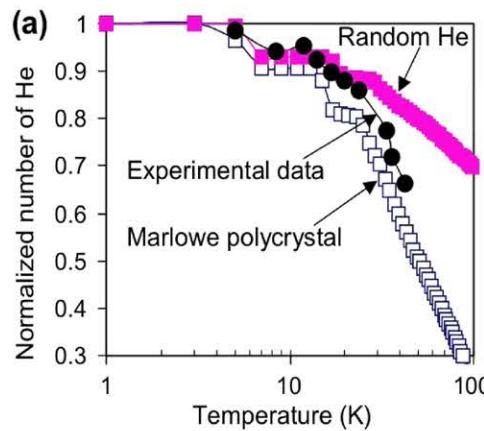
<sup>1</sup> Becquart et al. J. Nucl. Mater. 403, 75 (2010)

<sup>2</sup> M. Hou et al. J. Nucl. Mater. 403, 89 (2010)



# MMonCa simulation<sup>1</sup>

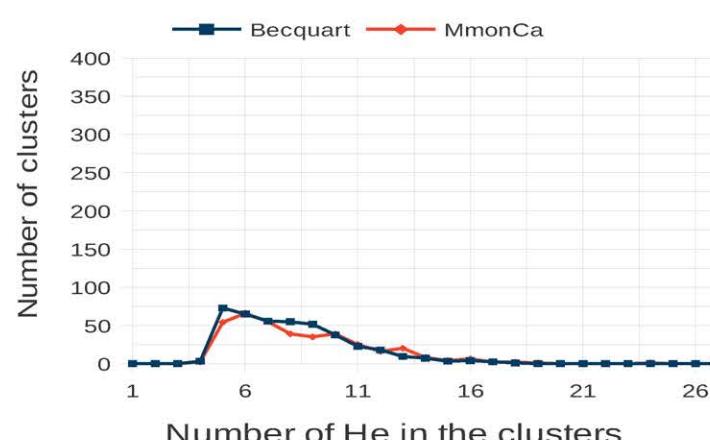
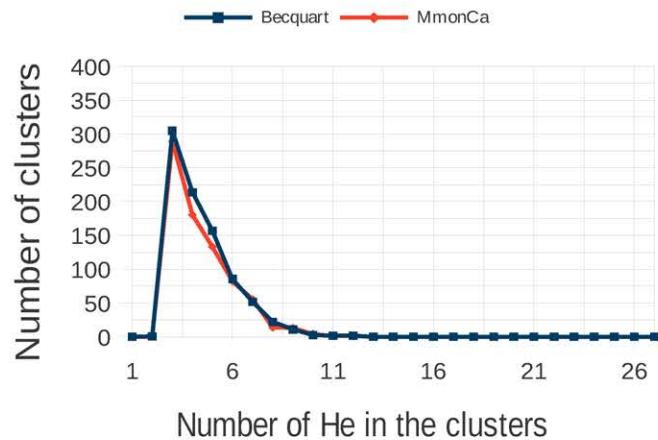
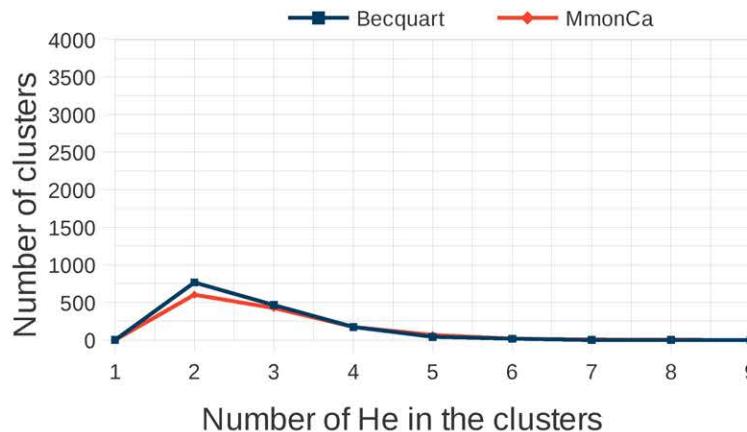
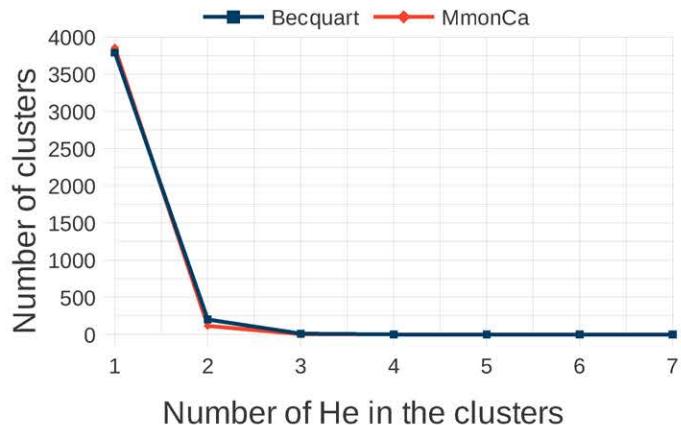
- Two implantations:
  - Sub-threshold at 400 eV (only He implantation)
  - Above-threshold at 3 KeV (He and FP implantation)
- Irradiated at 5K
- We followed the Marlowe implantation carried out by Becquart et al.
- Isochronal annealing for 60 s every 2K
- Simulation box: 317x126x126 nm<sup>3</sup>

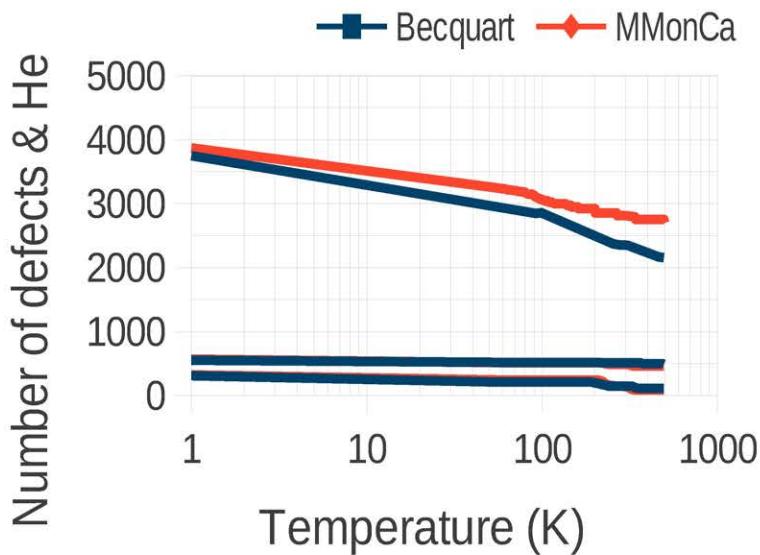


<sup>1</sup> Becquart et al. J. Nucl. Mater. 403, 75 (2010)  
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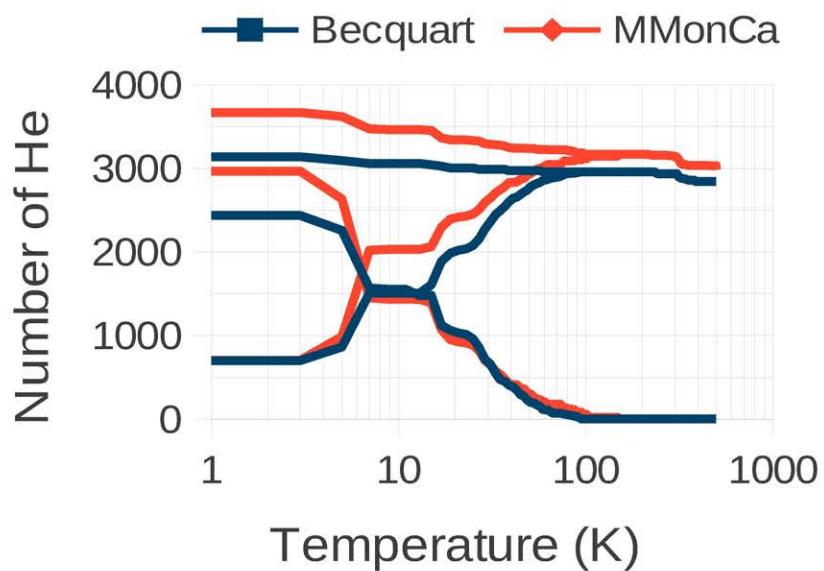


# MMonCa simulations Under-threshold





# MMonCa simulations Above-threshold



In the simulations:

- Interstitial/interstitial clusters move in 3D
- Capture radii not depends on the object



# Conclusions



Many thanks  
for  
your attention  
Questions?

Want to use MMonCa? Write to  
[ignacio.martin@imdea.org](mailto:ignacio.martin@imdea.org)

The screenshot shows the Eclipse C/C++ IDE interface with the following details:

- Project Explorer:** Shows the project structure under "MMonCa".
- LatticeAtom.h File:** Opened in the editor, containing C++ code for a lattice atom class.
- Build Log:** Shows the build process for configuration "Release" of project "MMonCa".
- Bottom Status Bar:** Displays "Writable" and "Smart Insert" status.
- Page Number:** "337 : 10" at the bottom right.