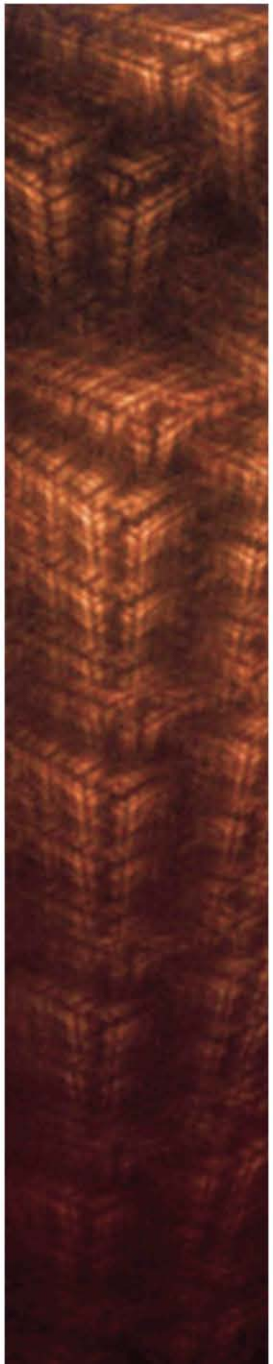

MMonCa: A flexible and powerful new Kinetic Monte Carlo Simulator

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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

Start

- 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 $R = \Sigma r_i$

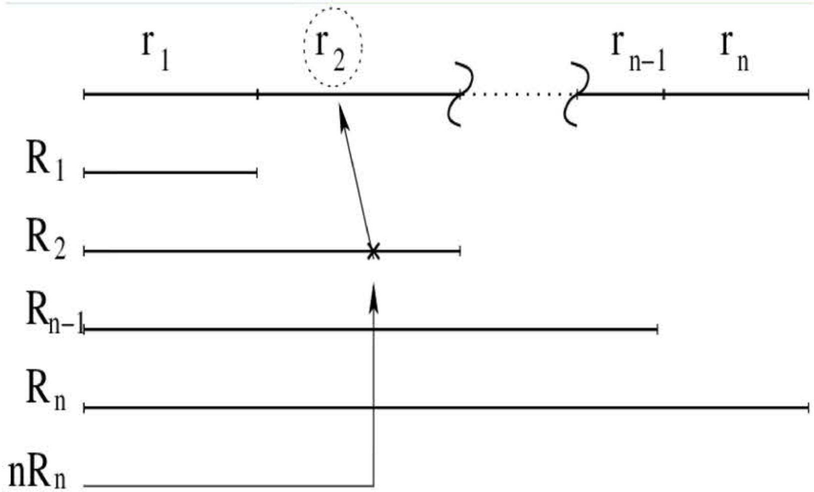
generate a random number $n \in [0,1)$

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

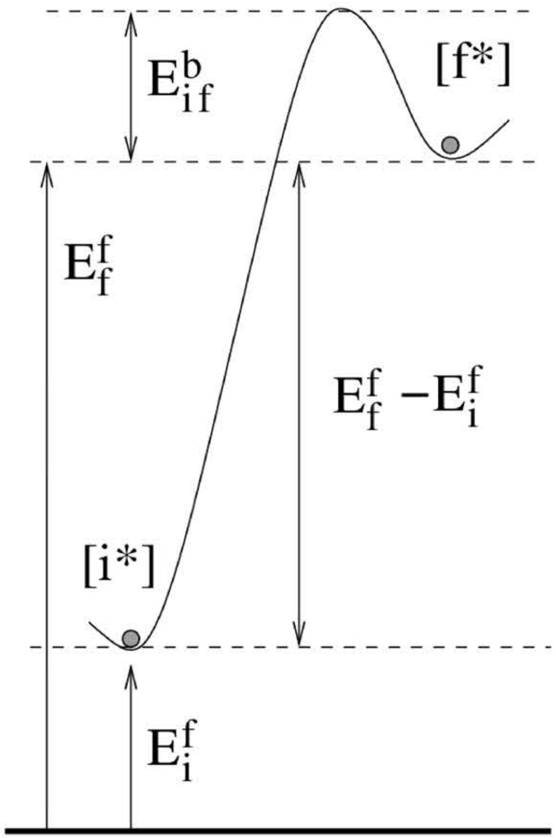
End



Object KMC: Rates

- All different rates are assume 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)



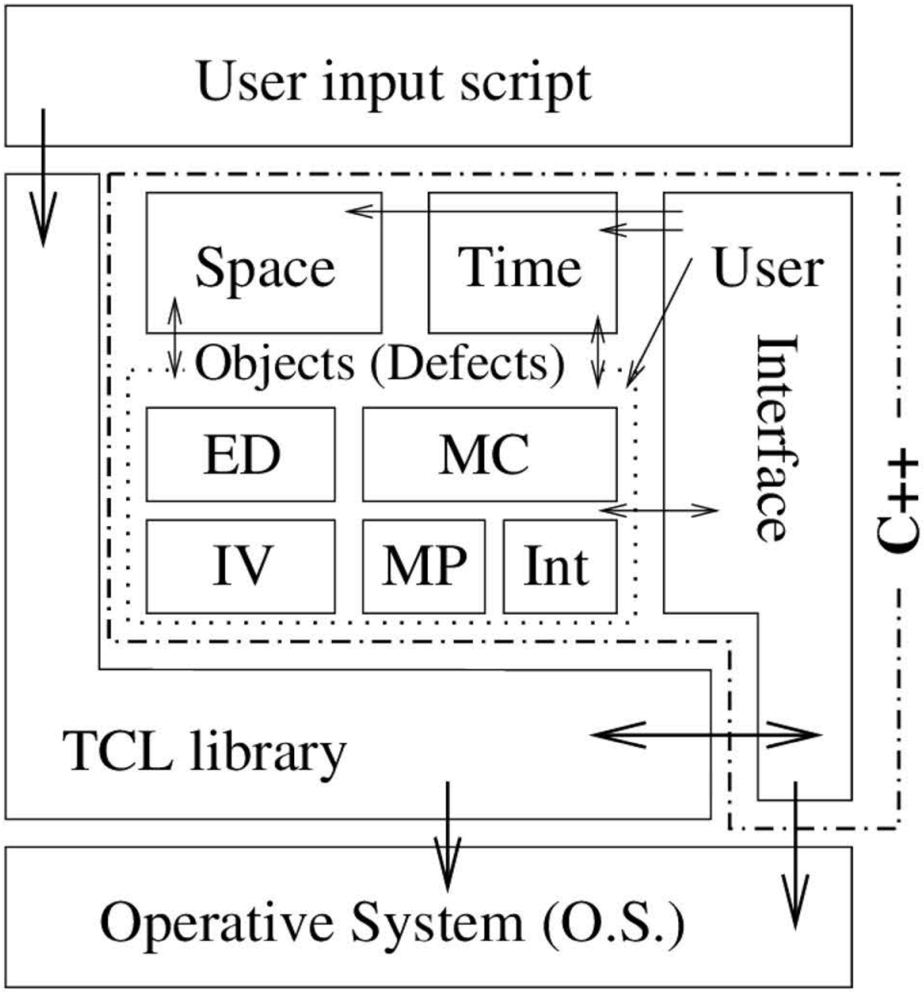
$$E_{ij} = E^f_j - E^f_i + E^b_{ij}$$

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

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).

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OKMC mechanisms

- Diffusion
  - I, V, C, He, …
  - He_nV_m, …
  - I_n, V_m, …
- Cluster emission
  - $He_nV_m \leftrightarrow He_{n-1}V_{m-1} + HeV$
  - $He_nV_m \leftrightarrow He_{n-1}V_m + He$
  - $He_nV_m \leftrightarrow He_nV_{m-1} + V$
  - $He_nV_m \leftrightarrow He_{n-1}V_{m+1} + I$
- Very complex clusters
  - $He_nC_mV_o \leftrightarrow He_nC_{m-1}V_o + C$
  - ...
- Extended defects
  - $I_n \leftrightarrow I_{n-1} + I$
  - I_n (A) $\leftrightarrow$ I_n (B)
  - I_n + Trap (mobile) $\leftrightarrow$ I_n Trapped (immobile)
- Damage
  - $I_nV_m \rightarrow I_{n-1}V_{m-1}$
- Interfaces
  - MP^A + A/B $\leftrightarrow$ MP(A/B) $\leftrightarrow$ MP^B + A/B
  - MP + A/B $\leftrightarrow$ A/B
  - ED + A/B $\leftrightarrow$ A/B
  - MC + A/B $\leftrightarrow$ A/B
  - Int $\rightarrow$ 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"
}
```

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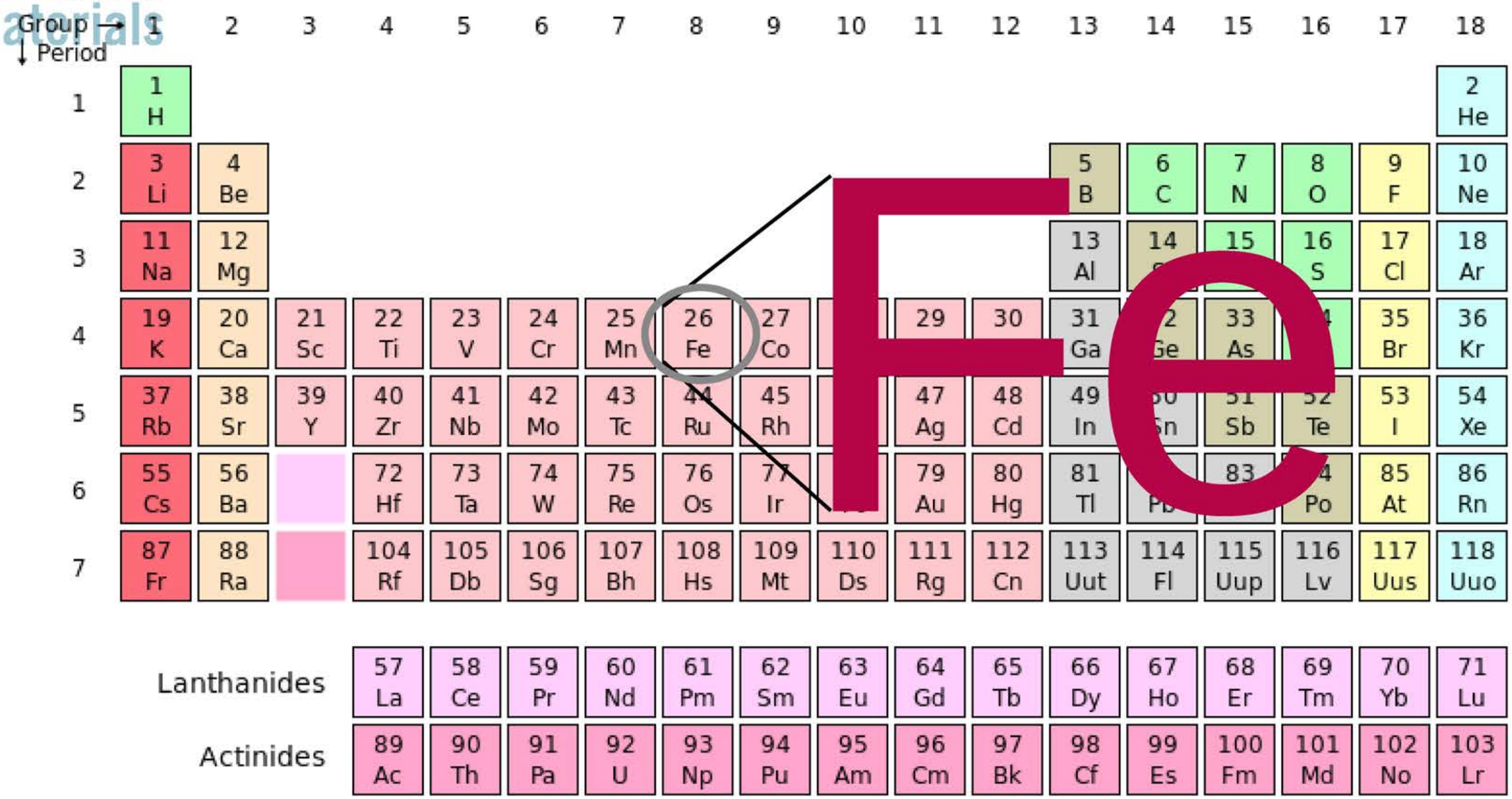

Isochronal annealing of α-Fe

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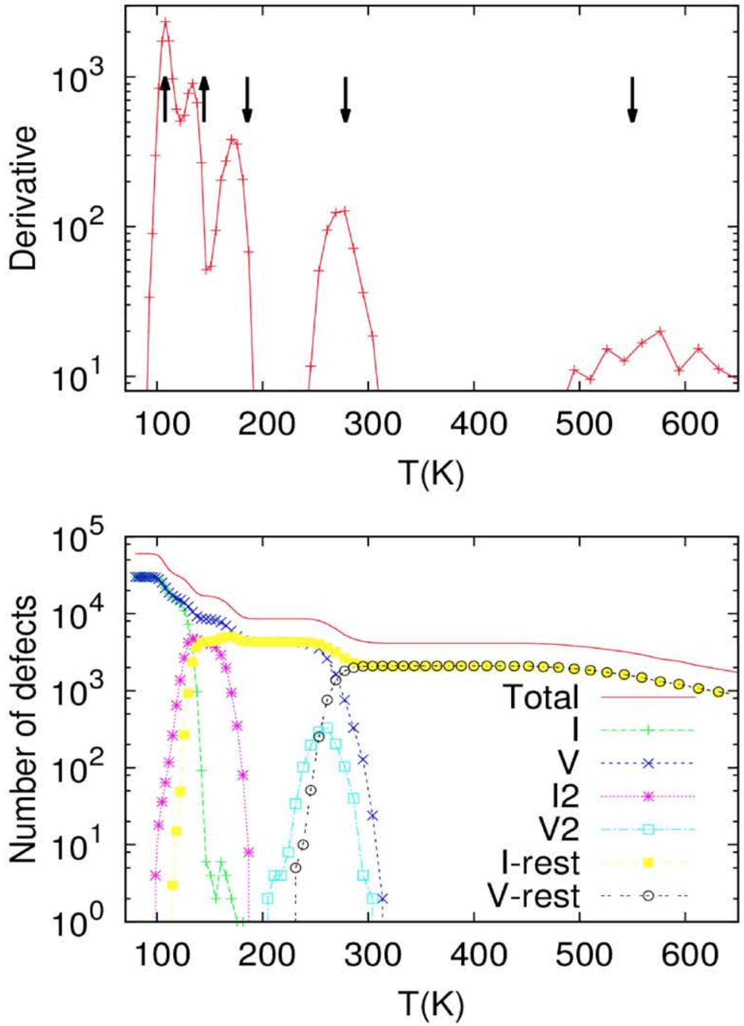
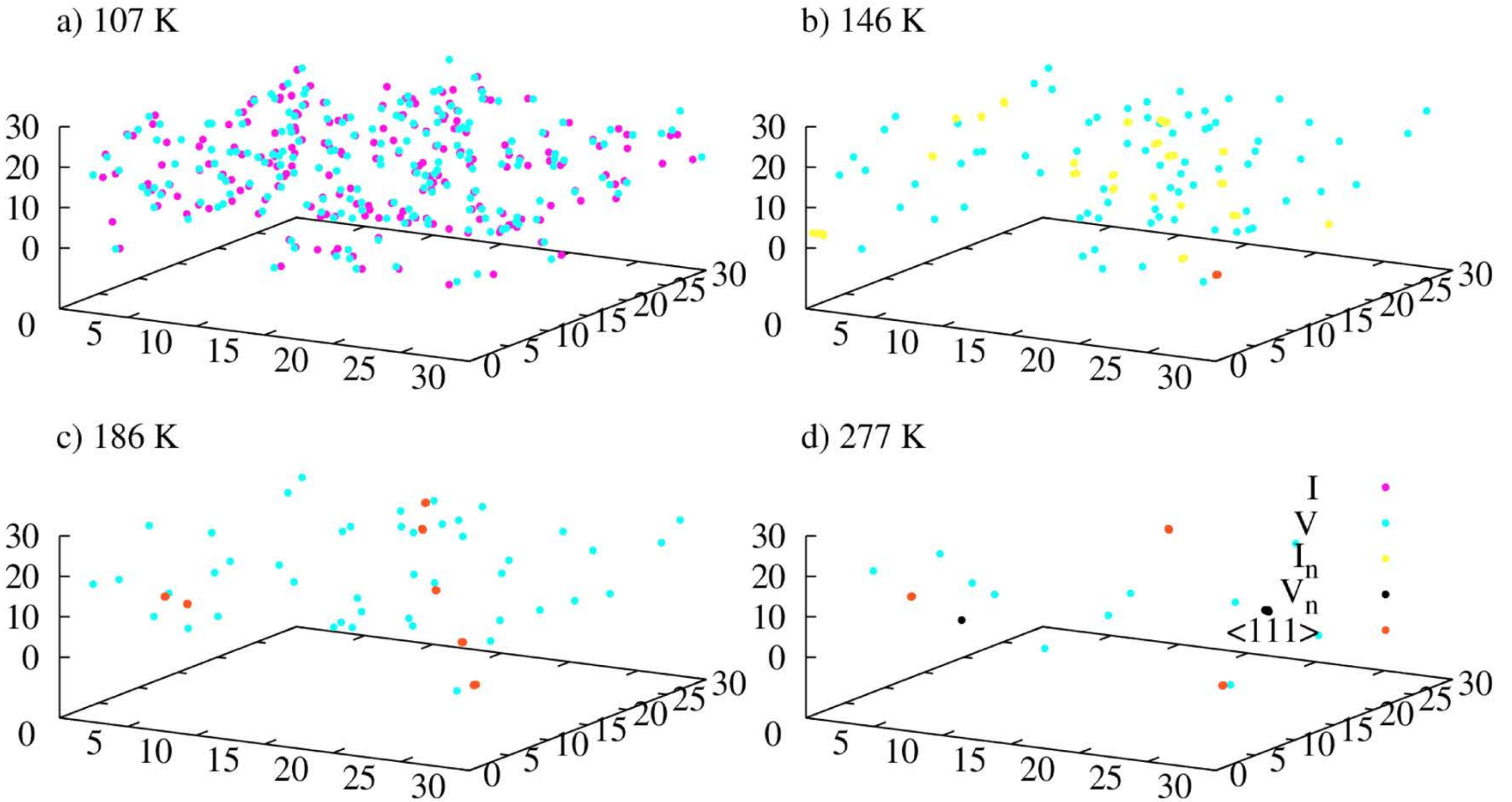
Defects and resistivity recovery during α-Fe annealing

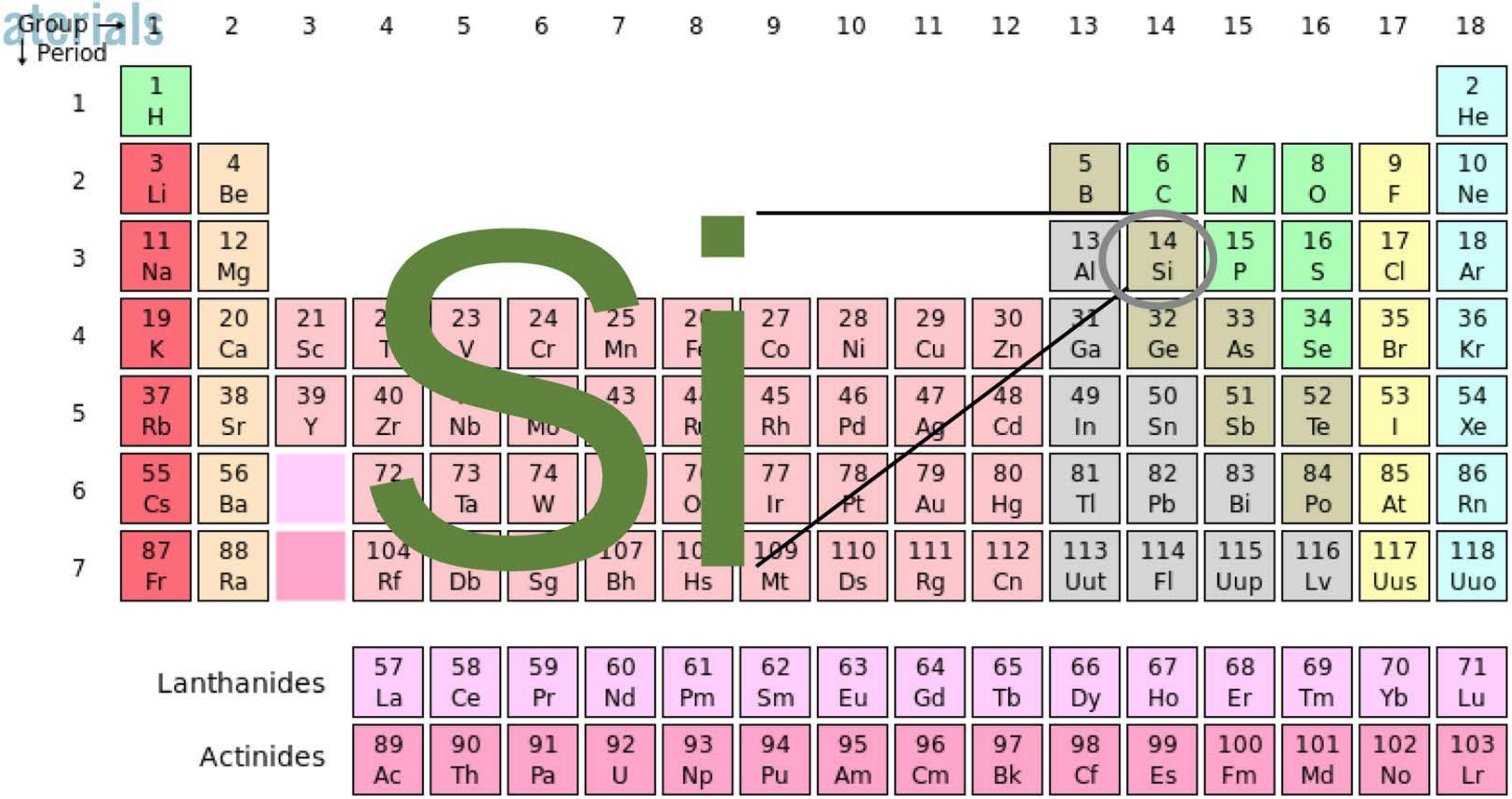


- Simulated isochronal annealing of 2e-4 dpa irradiated Fe.
- Excellent agreement with experiments[1] and simulations.[2,3]

[1] Takaki et al. Radiation Effects 79, 87 (1983)
[2] Fu et al. Nature materials 4, 68 (2005)
[3] Ortiz and Caturla. Phys. Rev. B 75, 1884101 (2007)

Defect population evolution during annealing of α-Fe





Annealing of implanted defects in silicon

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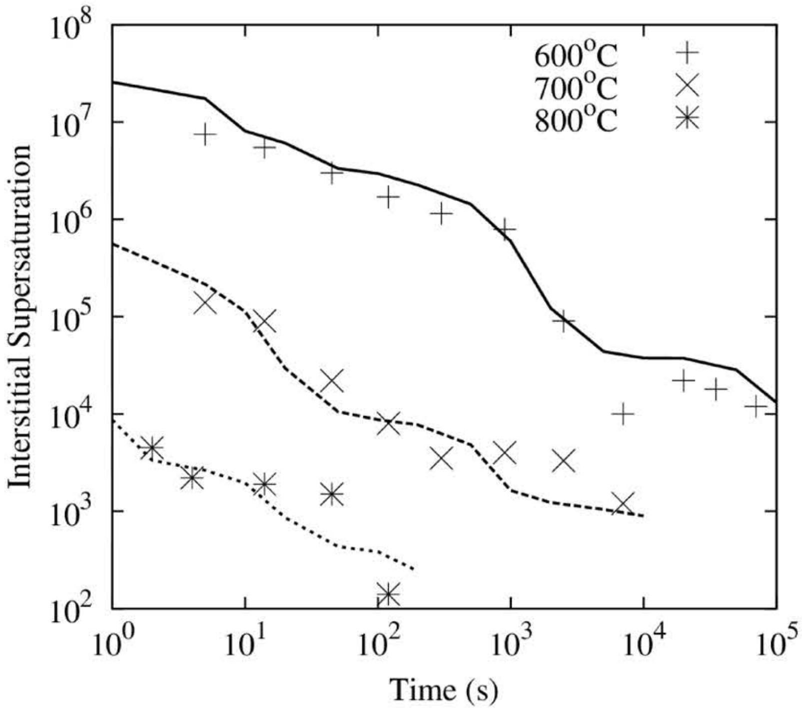
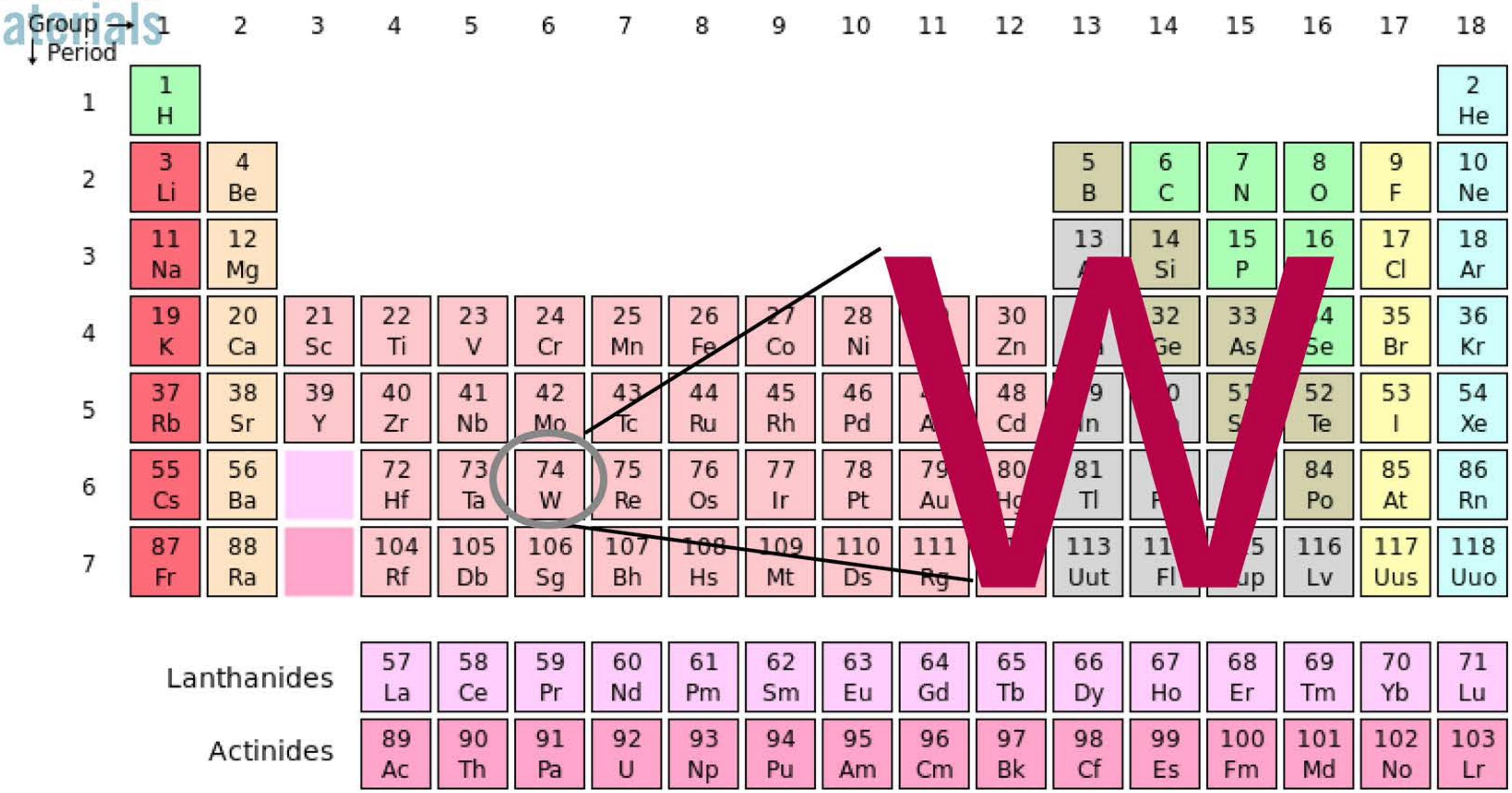
Interstitial evolution in damaged Si



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

[1] Cowern et al. Phys. Rev. Lett. 82, 4460 (1999)
[2] Martin-Bragado et al. Solid-State Electronics 52, 1430 (2008)



Evolution of damage in tungsten

MMonCa parametrization[1]

	Particles	Clusters
Mobile	He V I	He_n V_n I_n
Immobile	C (as traps for V, I)	He_nV_m He_nI_n CV_n, CI_n

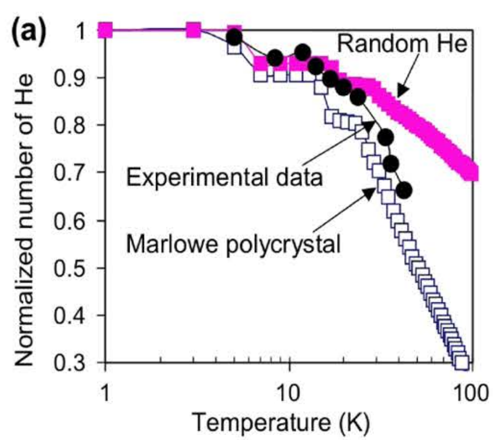
	He3
Epot	-2.39 eV
Emission pref. ($He_3 \rightarrow He_2 + He$)	9.9856e-4 cm2 s-1
Emig	0.05 eV
Migration pref.	9.9856e-6 cm2 s-1

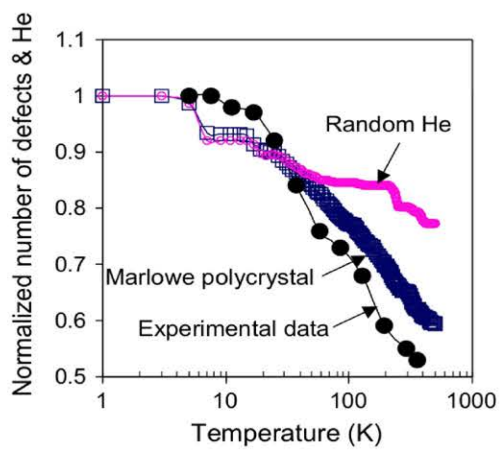
- Clusters defined by:
  - Potential energy
  - Emission prefactor
  - Migration prefactor
  - Migration energy
- The particle-cluster binding energy is calculated by MmonCa

[1] Becquart et al. J. Nucl. Mater. 403, 75 (2010)
[2] M. Hou et al. J. Nucl. Mater. 403, 89 (2010)

MMonCa simulation[1]

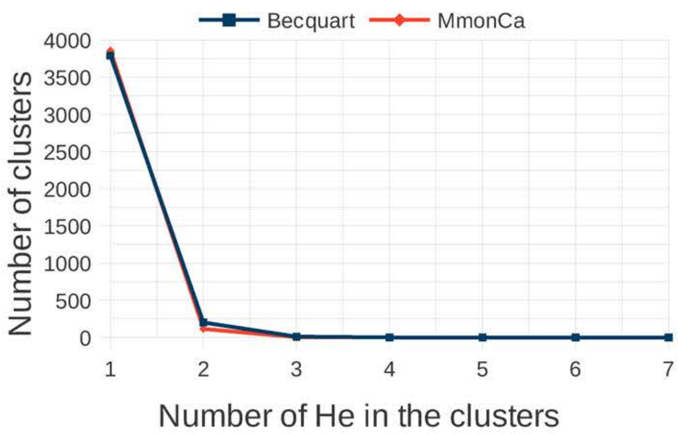
- Two implantations:
  - Sub-threshold at 400 eV (only He implantation)
  - Above-threshold at 3 KeV (He and FP implantation)
  - Irradiated at 5K
  - We followed the Marlowe implantation carried out by Becquart et al.
- Isochronal annealing for 60 s every 2K
- Simulation box: 317x126x126 nm^3

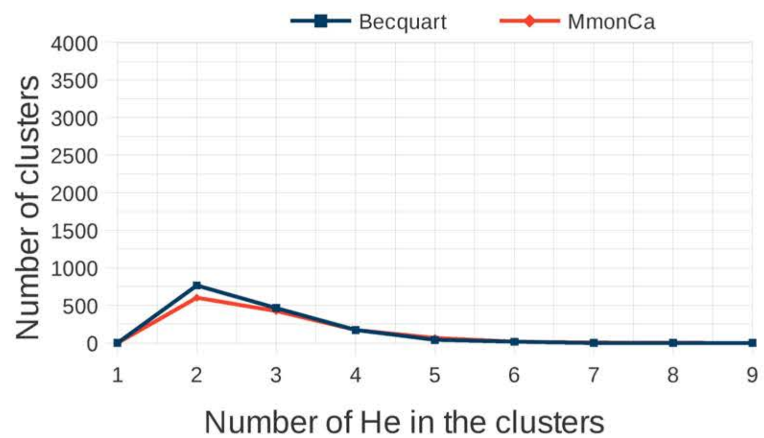


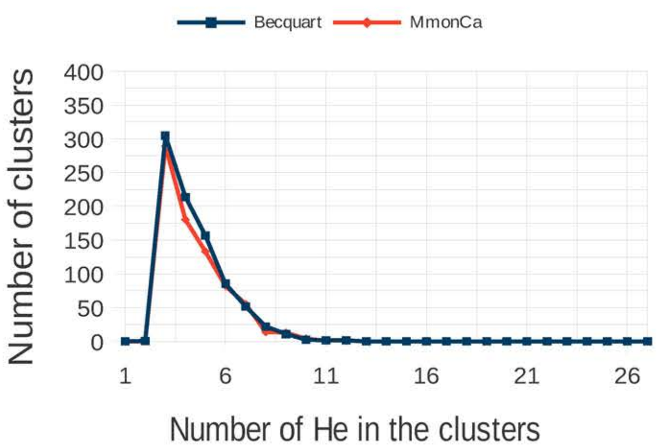


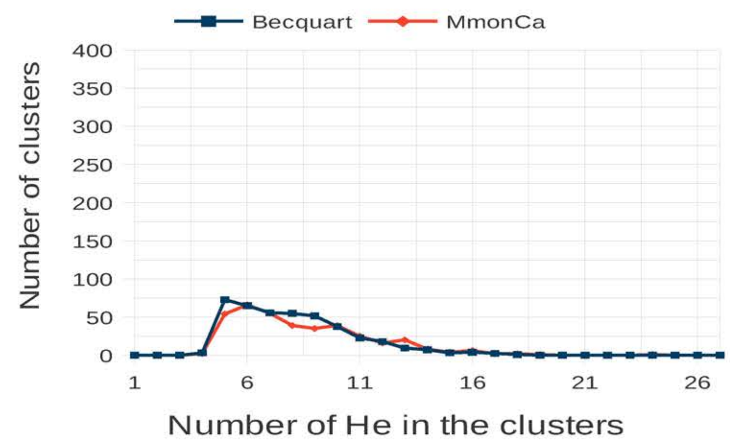
[1] Becquart et al. J. Nucl. Mater. 403, 75 (2010)
[2] M. Hou et al. J. Nucl. Mater. 403, 89 (2010)

MMonCa simulations Under-threshold

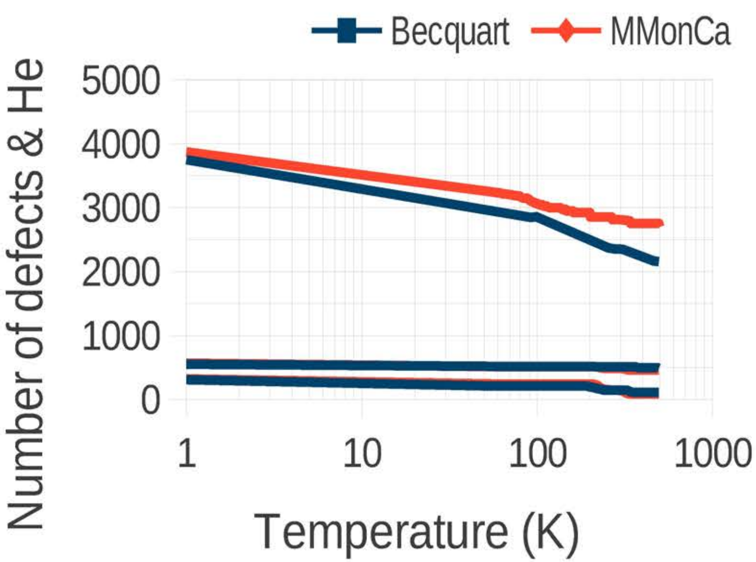


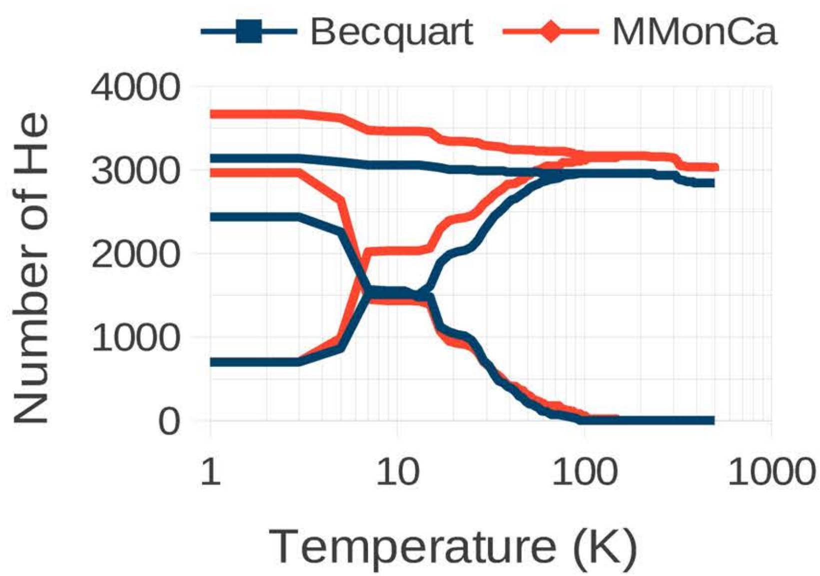






MMonCa simulations
Above-threshold





In the simulations:

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

Conclusions

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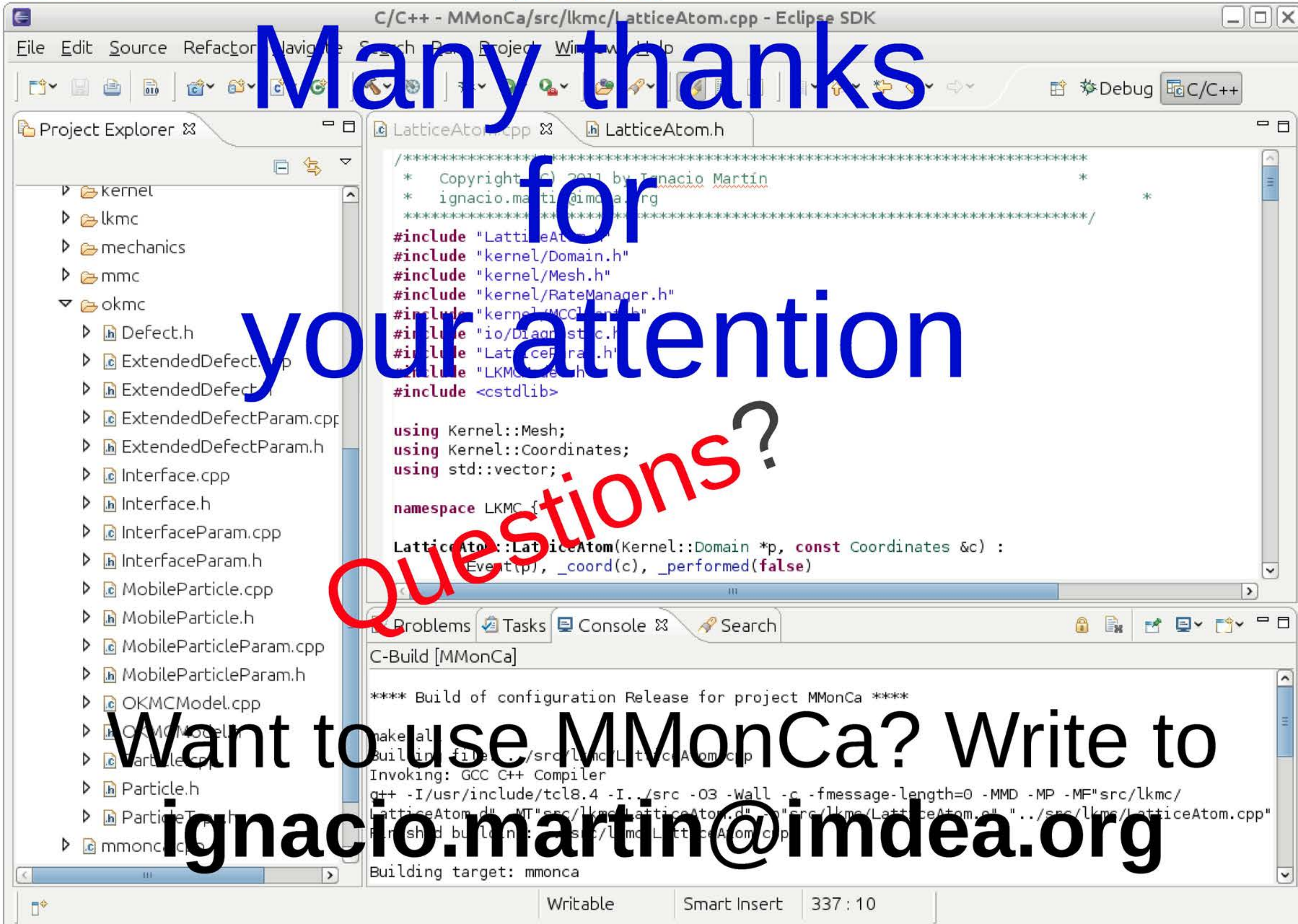

Many thanks for your attention

Questions?

Want to use MMonCa? Write to ignacio.martin@imdea.org