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Relating modeled positron response to experiment

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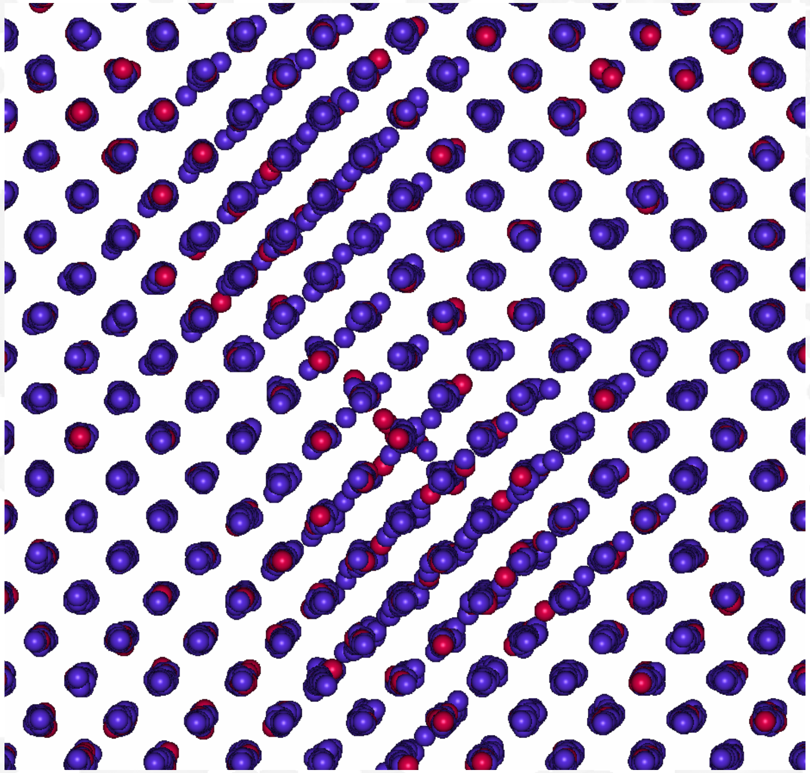
Outline

- Cascades in Fe-Cr system
- Fe-Cu system
- Conclusions

Cascades in Fe-Cr system

- 2, 10, 15 and 20 keV cascades studied (produced in SCK•CEN, Mol) using an EAM potential.



20 keV cascade

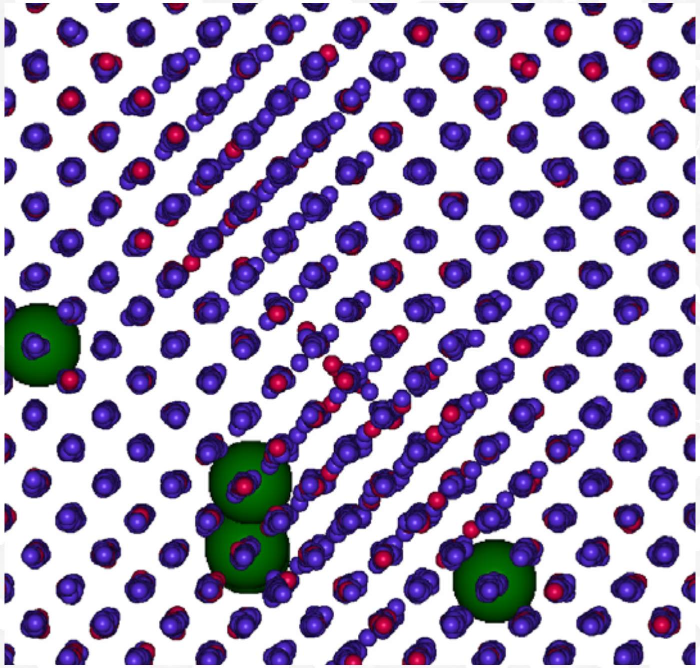
defect structure described in D.A. Terentyev et al., JNM **349** (2006) 119

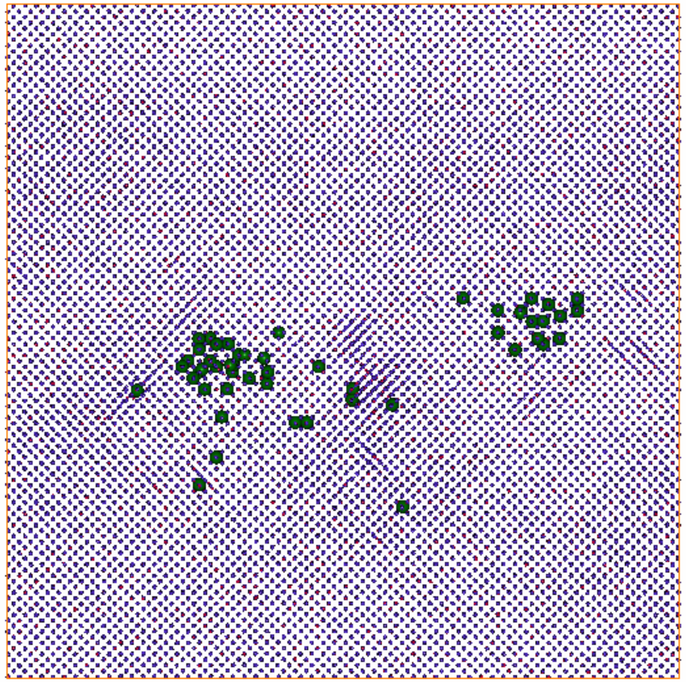
Cascades in Fe-Cr system

- Free volumes in simulation boxes are found using an automated procedure:
  - a regular 3D mesh (spacing 0.3 Å) is created inside the box
  - all mesh points are scanned and those having distance larger than 1.7 Å to all atoms are marked
  - neighboring marked mesh points are joined and create an open volume defect in the lattice
  - a cut around each open volume defect is taken and parameters for positron calculations are generated
  - cuts corresponding to neighboring open volume defects are joined

Cascades in Fe-Cr system

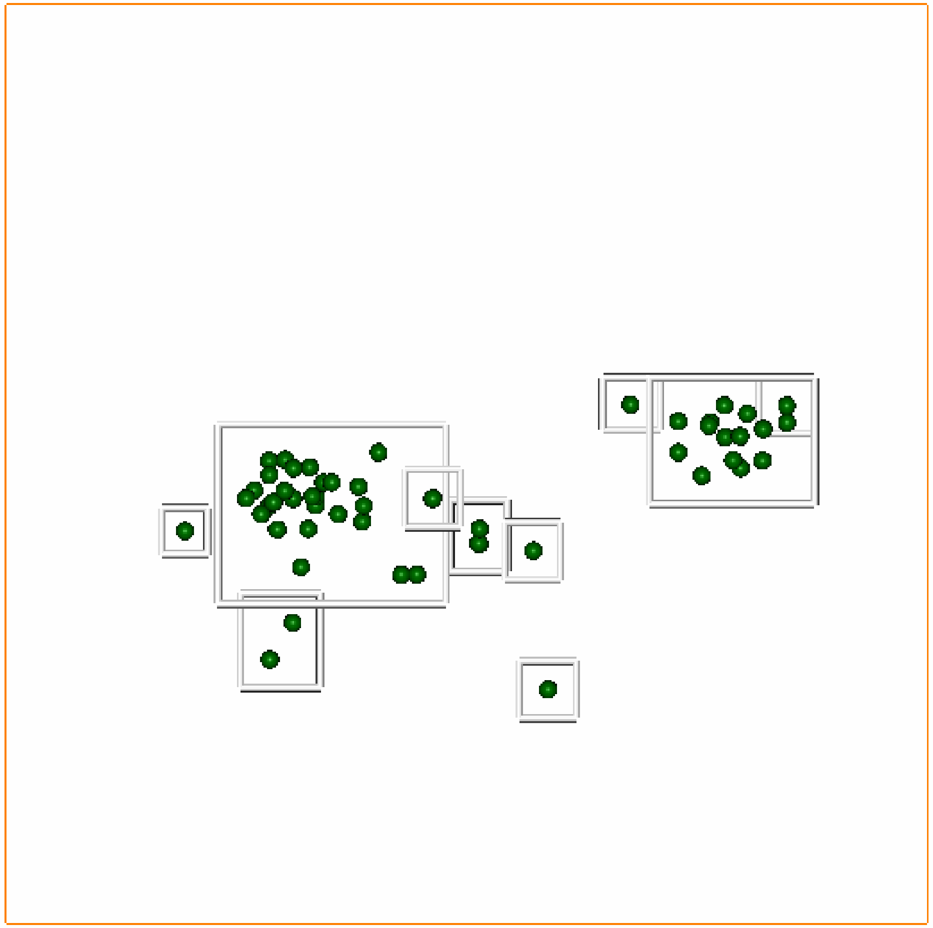
- Results of free volume analysis (20 keV cascade):





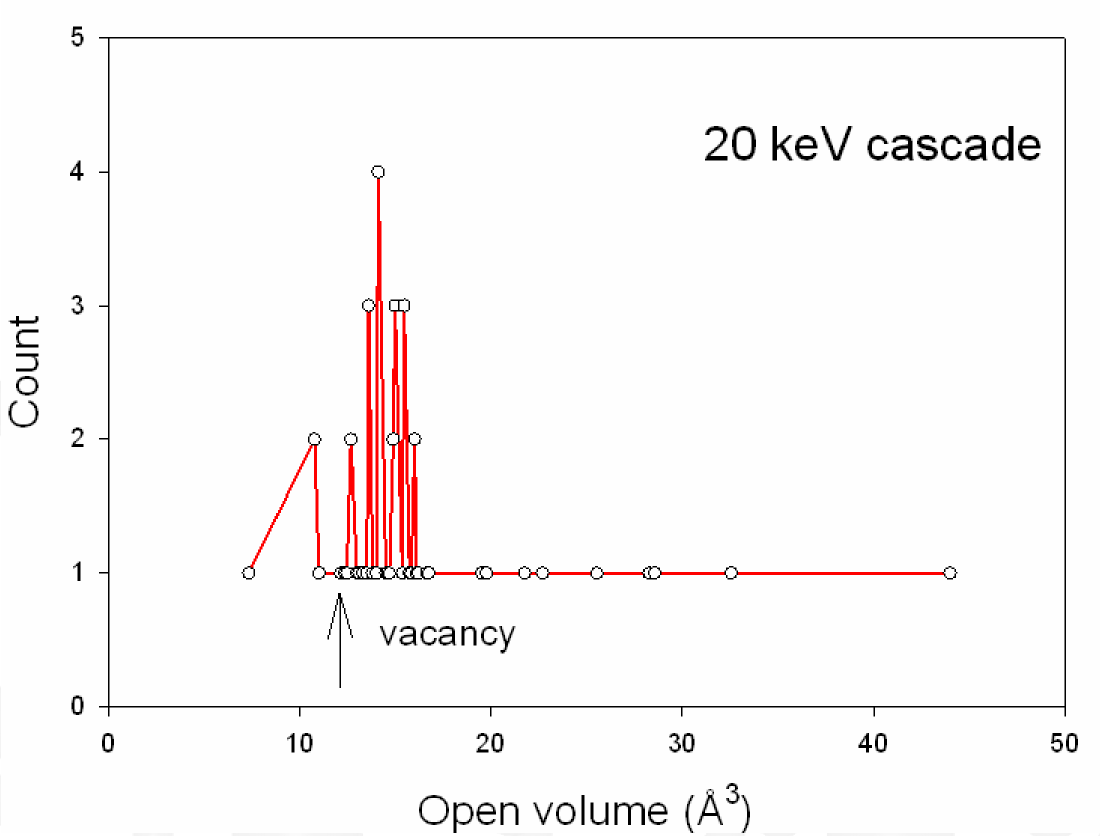
Cascades in Fe-Cr system

- Cuts around free volumes:



Cascades in Fe-Cr system

- Open volume distribution



positron lifetimes range from 150 to 220 ps

Cascades in Fe-Cr system

- The open volume analysis shows vacancies and small clusters.
- But under normal conditions vacancies are very mobile and are not stable.

Fe-Cu system

- Cu clusters in Fe represent a nice and simple system to study positron trapping to precipitates.
- PA experimental study by Y. Nagai et al., PRB **61** (2000) 6574.

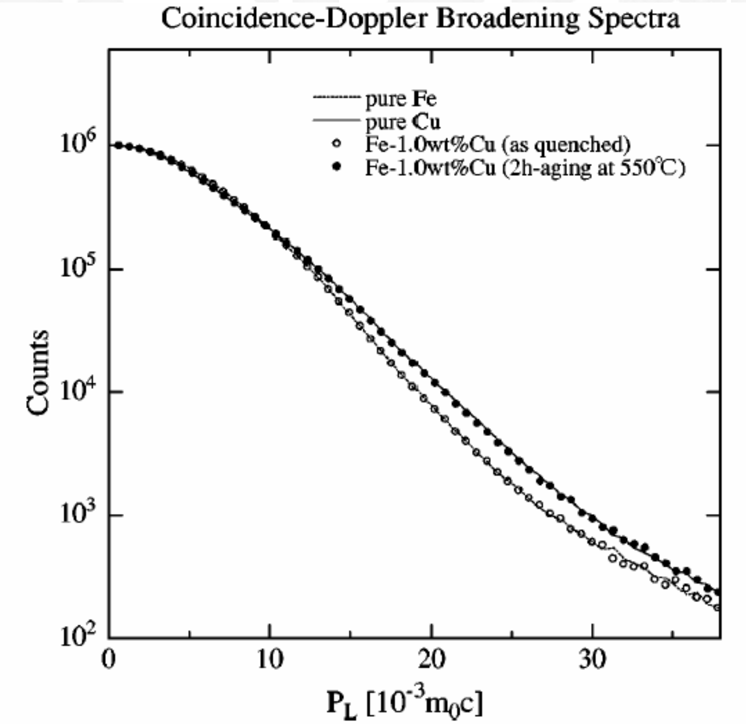
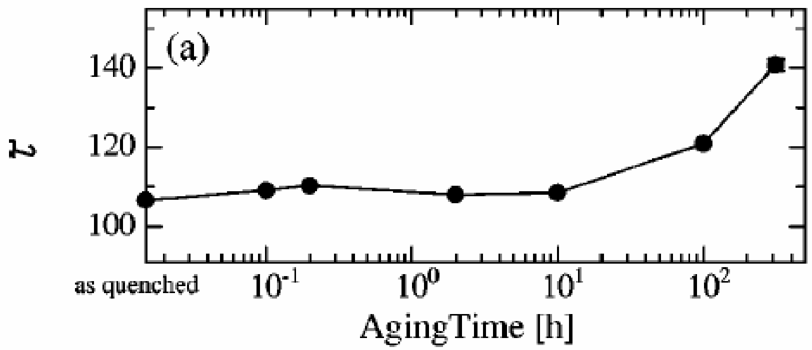


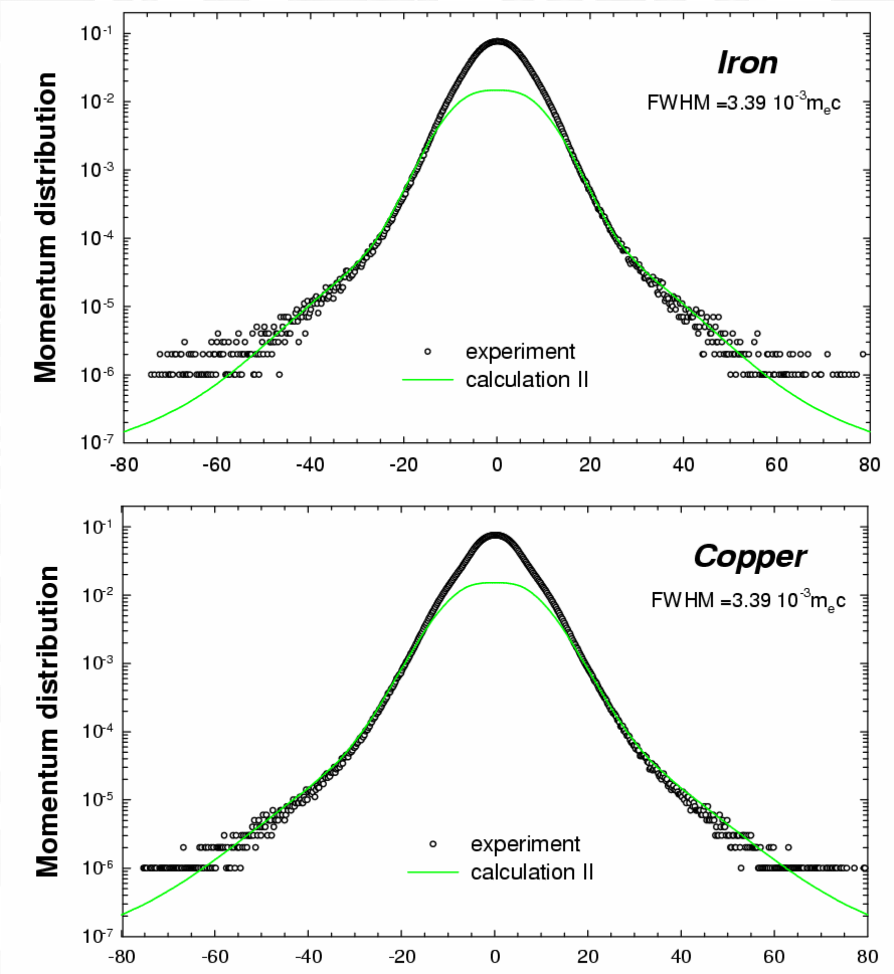
FIG. 1. CDB spectra for Fe-1.0 wt % Cu as quenched and after 2 h aging at 550°, compared with those for pure (bulk) Fe and Cu. Each spectrum is normalized to the same total count.



Aging dependence of positron lifetime.

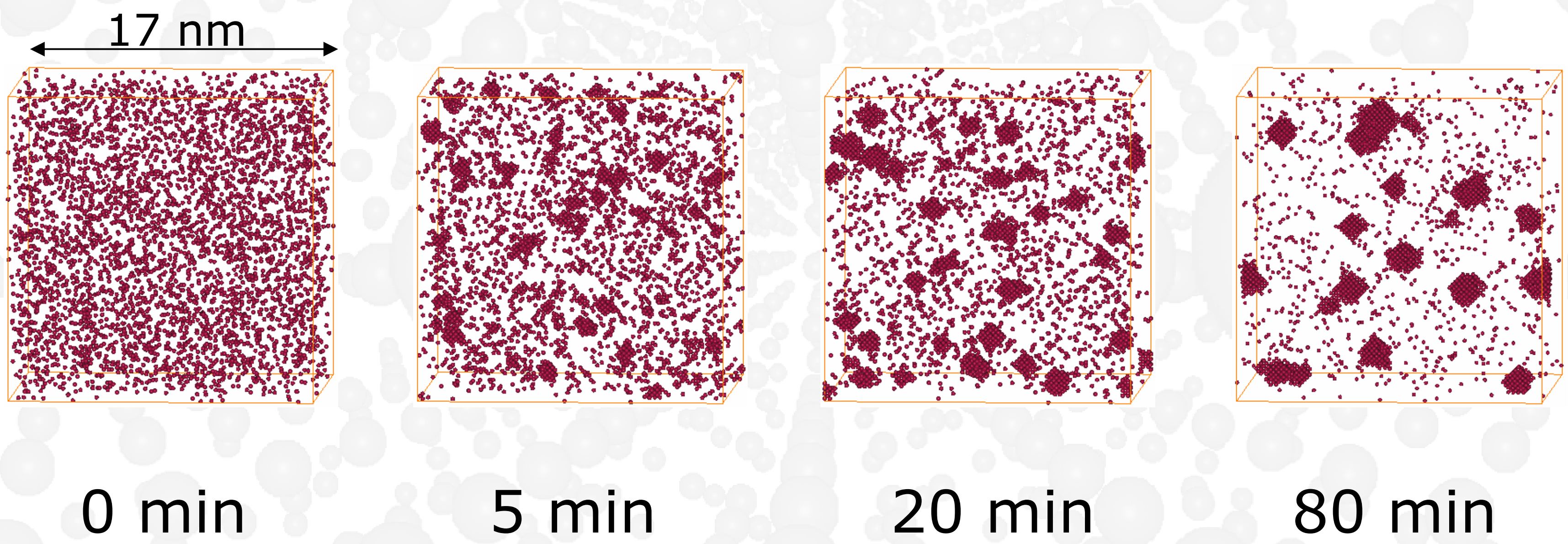
Fe-Cu system

- PA CDB experiment:
  - pure Fe, Cu – parameter 'tunning'



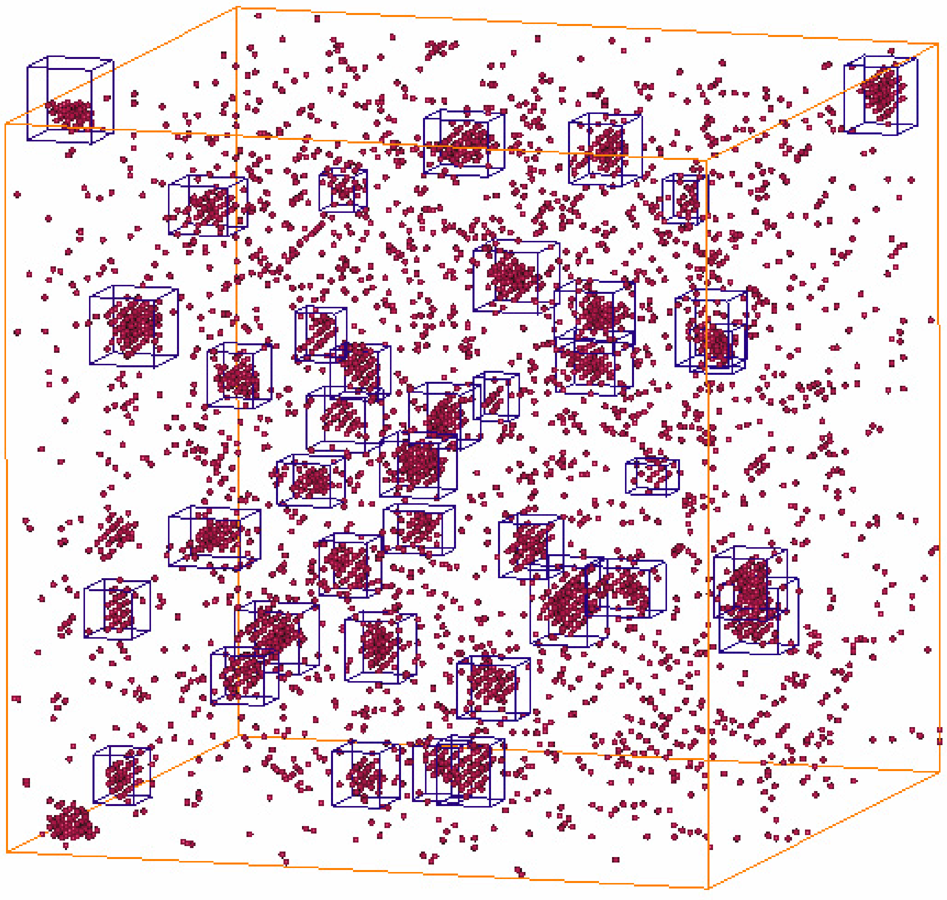
Fe-Cu system

- AKMC simulations (SCK•CEN, Mol)
  (1 at%Cu alloy, 60 × 60 × 60 bcc cells, 432000 atoms, 500 °C, Ludwig-Farkas potential, up to 6 × 10^9 steps, rigid lattice):



Fe-Cu system

- Simulations boxes too big for ATSUP:



Automatic routine how to select cuts around clusters.

- find all Cu atoms
- determine clusters by 1nn relationship
- make rectangular cuts around clusters
- cuts are `aligned' with the lattice

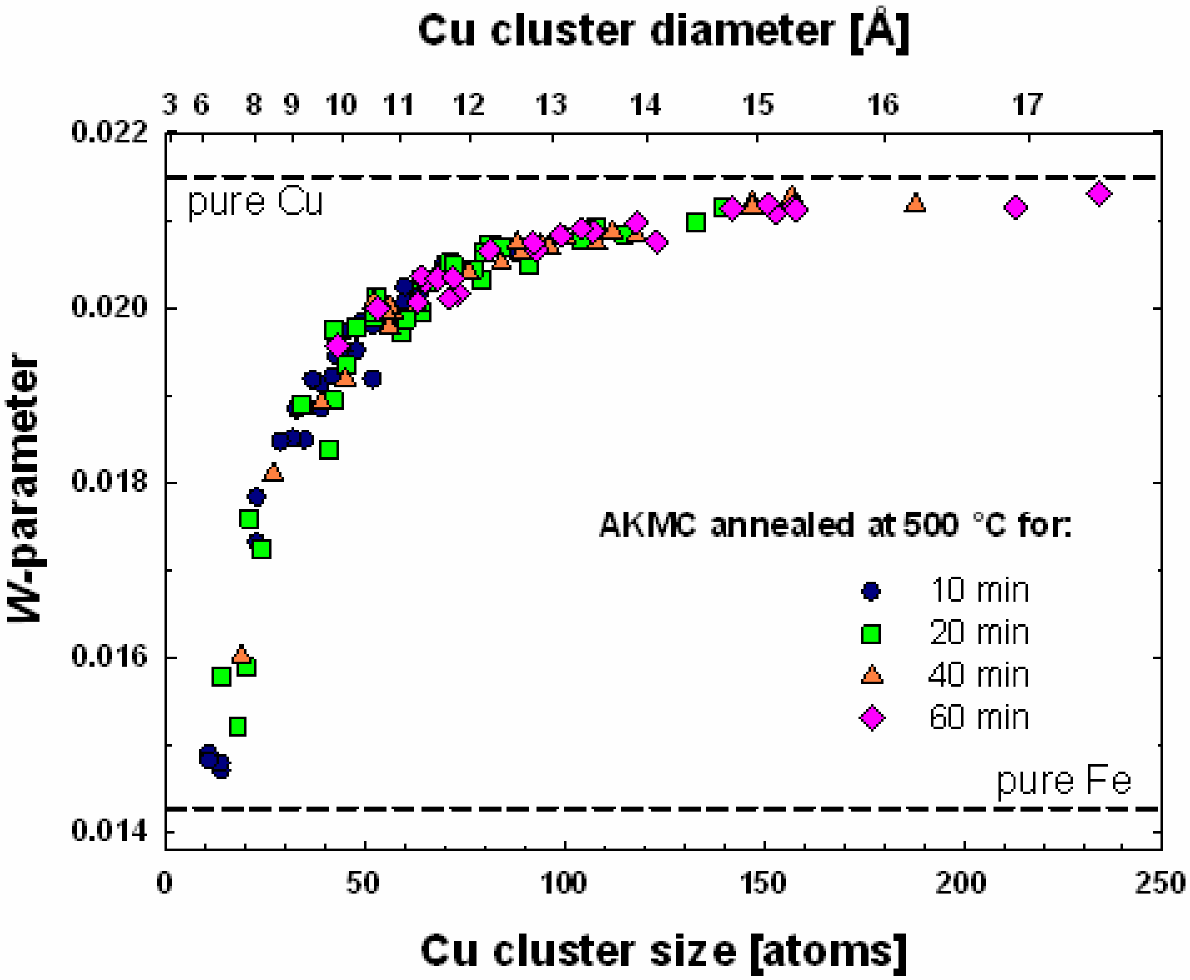
Fe-Cu system

- Calculation of *W*-parameter for all snapshopts

$$W = \int_{p_2}^{p_1} \rho(p)\, dp$$

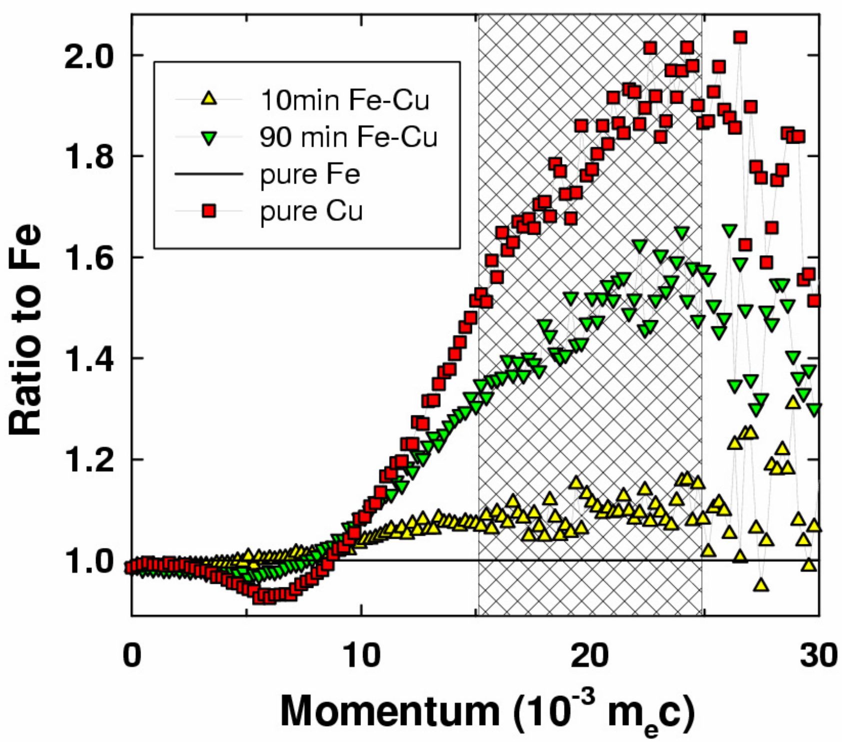
$p_1 = 15 \times 10^{-3}\ m_e c$

$p_2 = 25 \times 10^{-3}\ m_e c$



Fe-Cu system

- Simulation vs experiment: specific trapping rate estimate



- 10 min annealed sample

  $W_{exp} = 0.0153$

- $W_{exp} = (1-\eta)W_{Fe} + \eta\, W_{n\text{-}Cu}$

- Simulations:

  $n = 45$; $c = 9 \times 10^{18}$ cm^{-3}

  $W_{45\text{-}Cu} \approx 0.0195$

- $\eta \approx 21$ %

Fe-Cu system

- Simulation vs experiment: specific trapping rate estimate
  - Trapping rate:

    $\eta = \kappa / (\kappa + \lambda_{Fe}) \quad \rightarrow \quad \kappa \approx 2.5 \text{ ns}^{-1}$

  - Specific trapping rate:

    $\kappa = \nu c \quad \rightarrow \quad \nu \approx 2.8 \times 10^{-10} \text{ cm}^3/\text{s}$

  - Specific trapping rate for single vacancies in Fe:

    $\nu_{Fe\text{-}V} = 1.3 \times 10^{-8} \text{ cm}^3/\text{s}$

  - $\nu << \nu_{Fe\text{-}V}$ (transition limited trapping regime?)

Fe-Cu system

- Supposing the process is ‘diffusion limited’

  $\kappa = 4\pi RcD_+$ $(\nu = 4\pi RD_+)$

  using D_+ = 1.0 cm²/s and $R(45)$ = 5.0 Å

  we get

  $\kappa = 5.6 \times 10^3\ \text{ns}^{-1}$ $\nu \approx 6.3 \times 10^{-7}\ \text{cm}^3/\text{s}$,

  which strongly contradicts previous values and the process of trapping to Cu precipitates should be ‘transition limited’

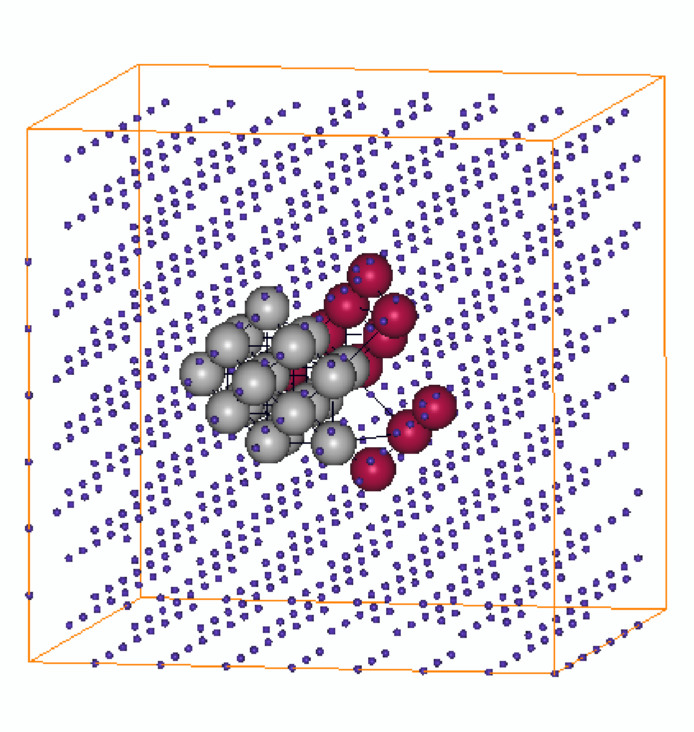
- In this way, the whole dependence

  ν*(annealing time)* = ν*(cluster size)*

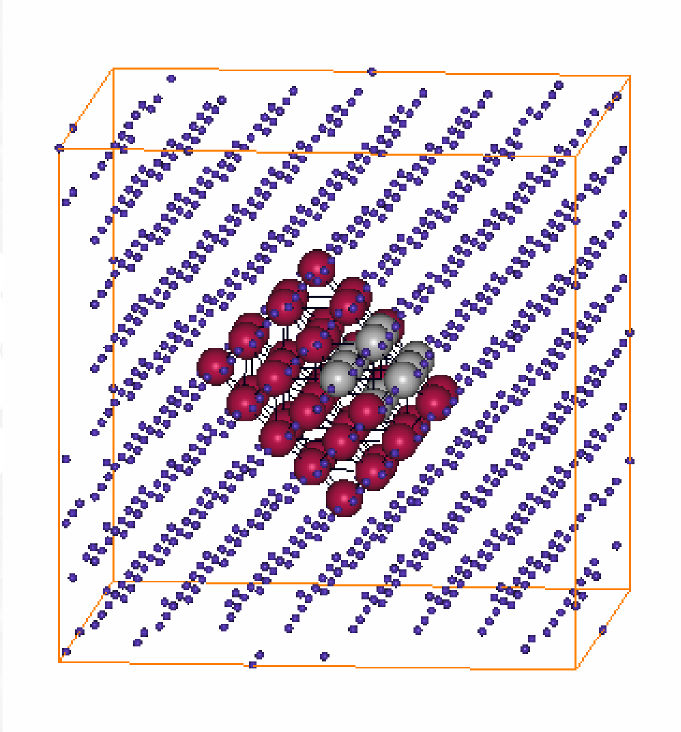
  could be evaluated.

Fe-Cu system

- Medium size Cu-V clusters have been also studied (simulations performed in SCK•CEN, Mol).



N(Cu)=10, N(V)=20

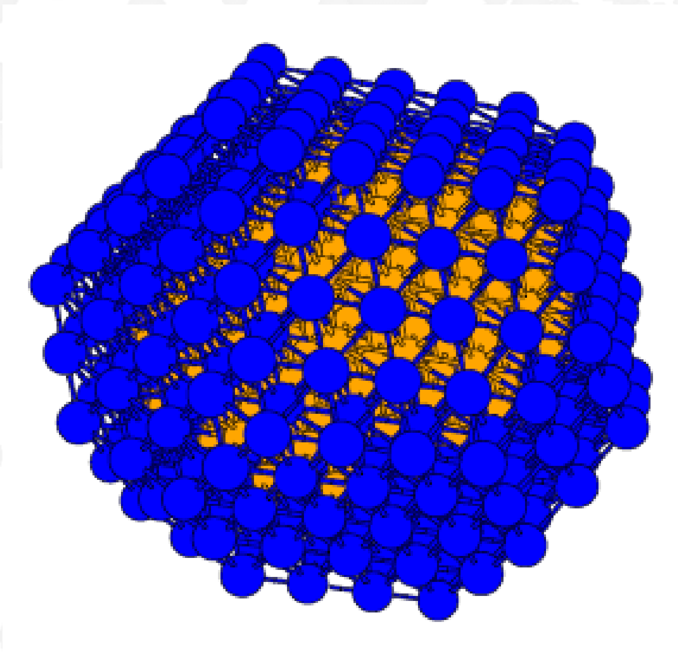


N(Cu)=40, N(V)=10

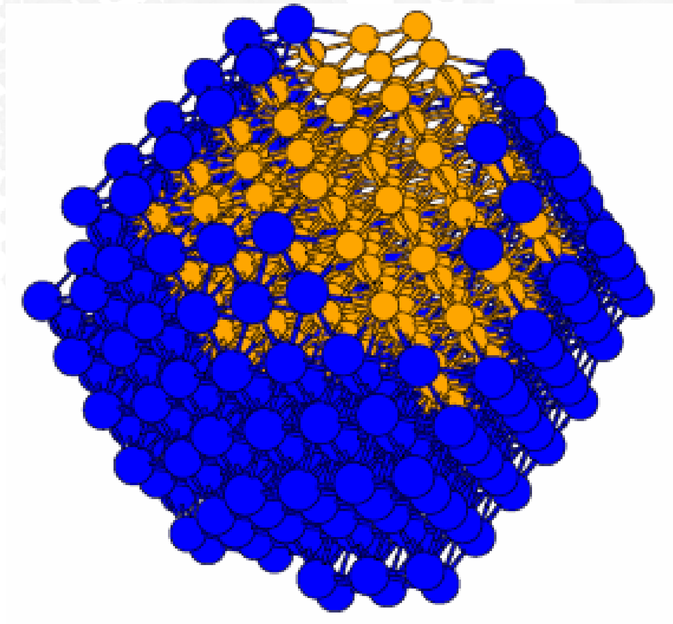
Fe-Cu system

- Complete vs incomplete ‘coverage’?

N(Cu) = 300, N(*V*) = 100



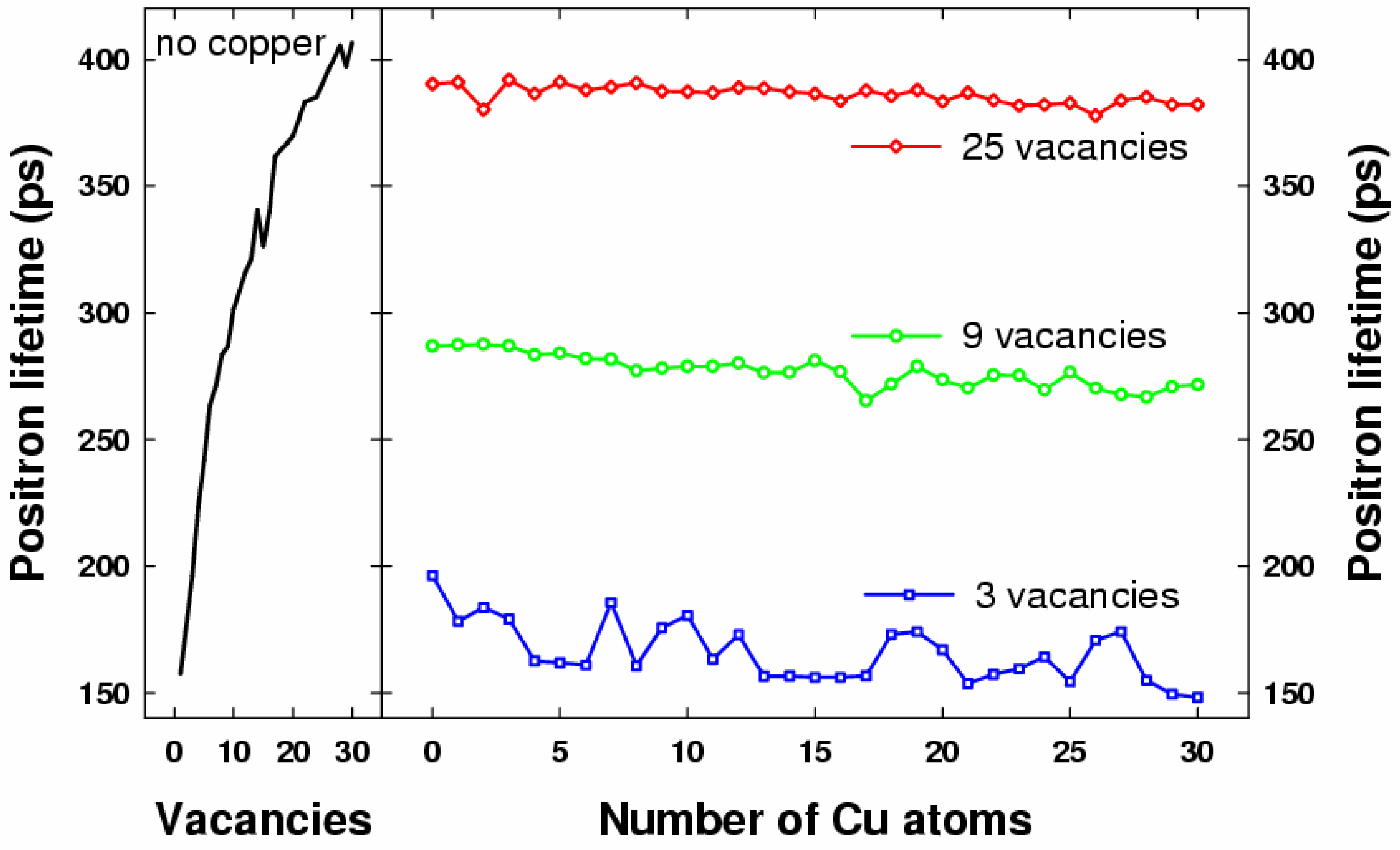
Ackland-Bacon



Ludwig-Farkas

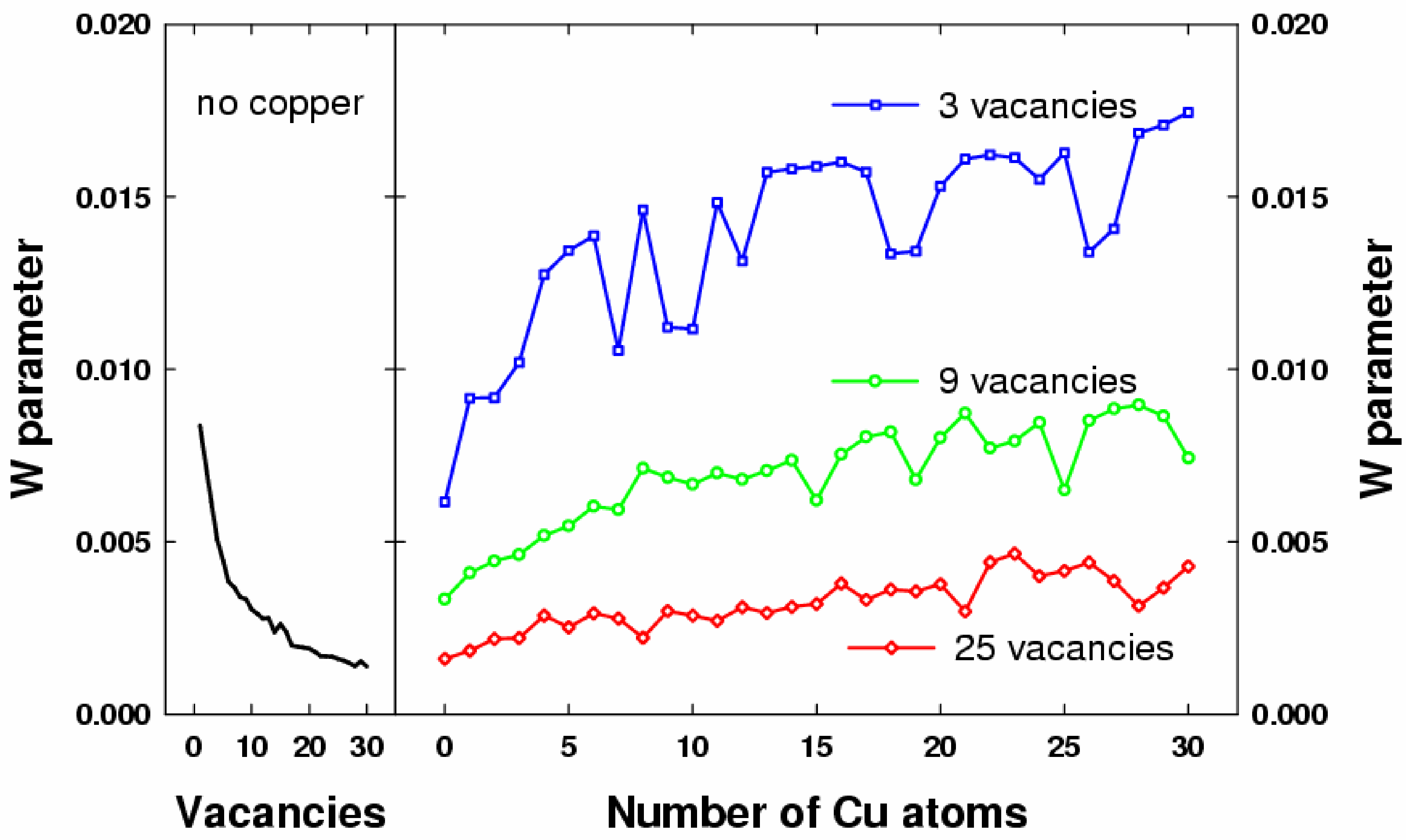
Fe-Cu system

- Calculated dependencies of lifetime on N(Cu) for given N(*V*).



Fe-Cu system

- Calculated dependencies of W-parameter on N(Cu) for given N(*V*).



Fe-Cu system

- Problems with simulations: in some cases there are two Cu-VC clusters in the simulation box.
- To our knowledge, there is no experimental study addressing the problem of Cu atoms in the vicinity of vacancy clusters.
- Further work is in progress.

Conclusions

- Irradiation does really produces vacancies and their clusters in Fe-Cr system.
- Calculated lifetimes agree with those seen in experiment.
- Cascades should be simulated considering realistic microstructure (dislocations, GBs, clusters, etc.).

Conclusions

- Cu precipitations in Fe can be effectively studied with positrons.
- The question of positron trapping into Cu clusters requires further study.
- By combining structure simulations, positron simulations with experiment, average cluster size can be determined.
- The problem of vacancy cluster decoration with Cu atoms can be also addressed with the help of simulations.

Thank you!