Radiation Damage and Multiscale Modeling Activities At Lawrence Livermore National Laboratory

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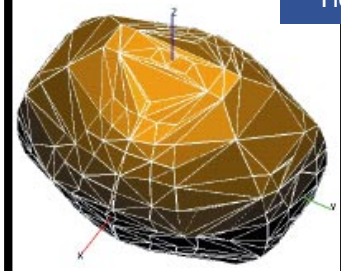
Aggressive multiscale materials modeling program at LLNL

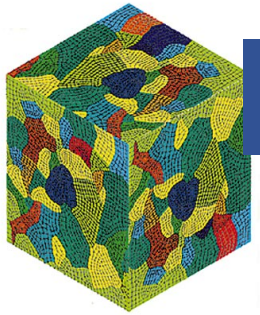
Continuum

Yield surface



ALE3D

Mesoscale

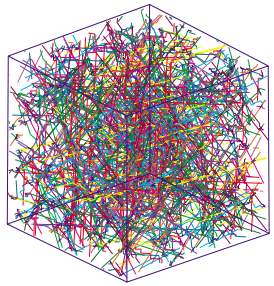


Single crystal constitutive relation

NIKE3D

Successful implementation requires closely coupled experiments and models

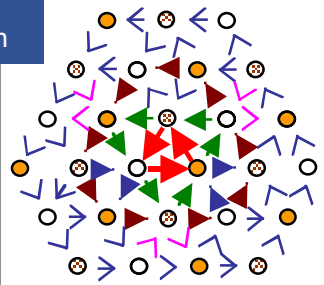
Microscale



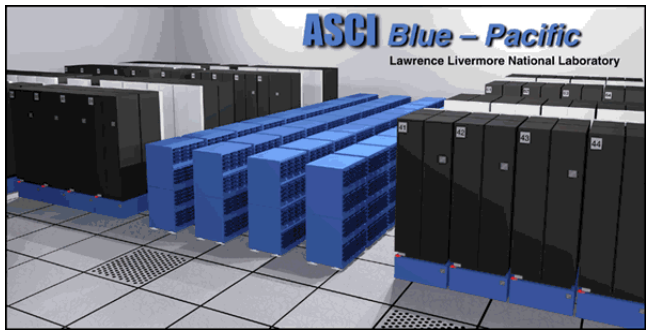
Rules for dislocation motion and multiplication

Dislocation Dynamics

Atomic Scale



Molecular Statics and Dynamics



Computational Materials Science Group (16 + 1 student)

- Electronic structure theory (4)
  - Tony Gonis, Babak Sadigh, Mike Surh, Patrice Turchi

- Radiation damage & defect physics - atomistic modeling (6)
  - Eduardo Bringa, Maria Jose Caturla, Alison Kubota, Jaime Marian, Brian Wirth, Bill Wolfer

- Dislocation theory & mechanics (7)
  - Tom Arsenlis, Maria Bartelt, Vasily Bulatov, Wei Cai, Maurice DeKonig, Chris Krenn, James Stolken

<u>Unique capabilities:</u>

- Atomistic simulations of radiation damage, cascade aging, kinetic Monte Carlo
- Large scale molecular dynamics of dislocation interactions
- Large scale dislocation dynamics

- Experimental: positron annihilation spectroscopy (3)
  - Palakkal Asoka-Kumar, Phil Sterne, Rich Howell

Radiation damage activities at Livermore

- ASCI Stockpile Stewardship:
  Aging (Wolfer) and Dynamics of Metals (Chandler & Diaz de la Rubia)

- Fusion materials:
  MFE (OFES, Wirth)
  IFE (DP, Caturla)
  Defect - grain boundary interactions (LDRD, Kubota, Caturla and Wirth)

- Light water reactor materials:
  RPV embrittlement (LDRD, Wirth)
  Core internals - hardening and embrittlement (NEPO, Wirth)
  - swelling & creep, (NERI, Wolfer)
  Grain boundary engineering (NERI, King)

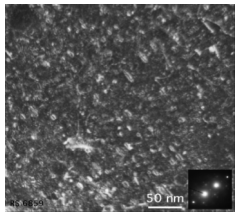
- GeV electron-positron targets at SLAC (LDRD, Caturla and Wirth)

Research strategy

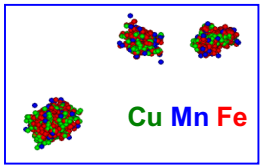
Experiment

Measure features

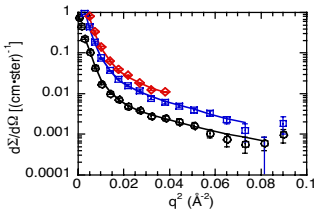
TEM



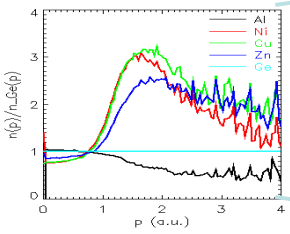
APT



SANS

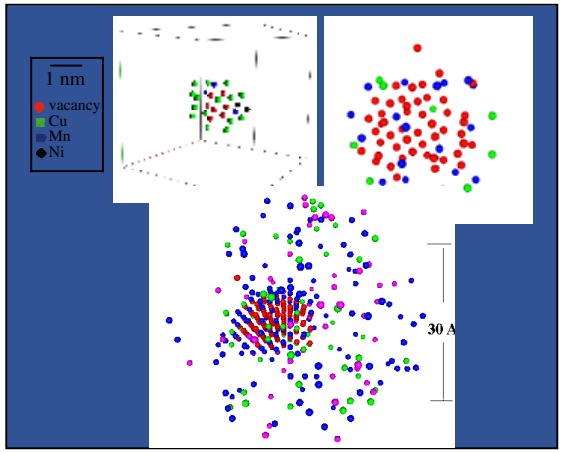


PAS



PAS group:
P. Asoka-Kumar
P.A. Sterne
R.H. Howell

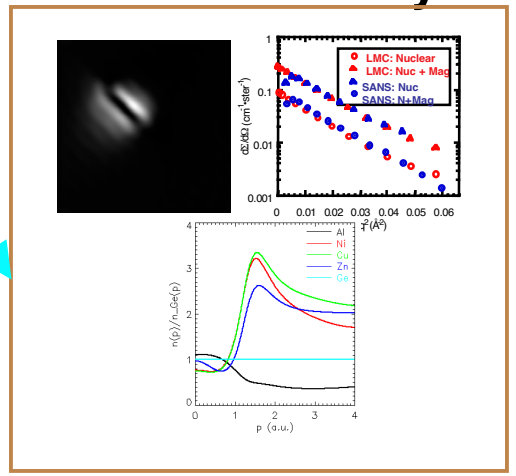
Multiscale modeling



fundamental understanding

Simulate observables

TEM, SANS, Positron theory



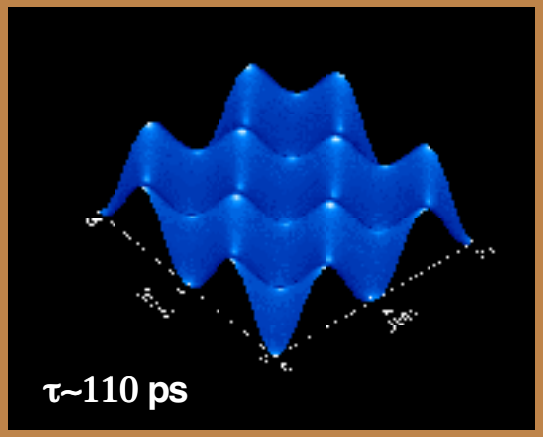
Predict features

Apply complementary experimental measurements, closely coupled to modeling and PAS/SANS/TEM theory

Positron annihilation spectroscopy

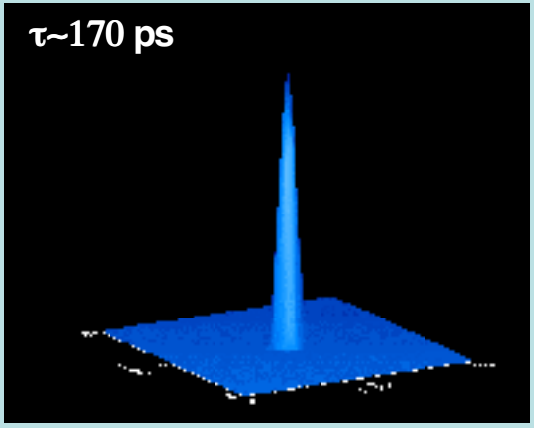
Positrons rapidly thermalize (within 5-10 ps) in metals. Thermalized positrons diffuse and localize ('trap') at defects before annihilation.

Bulk metal without defects

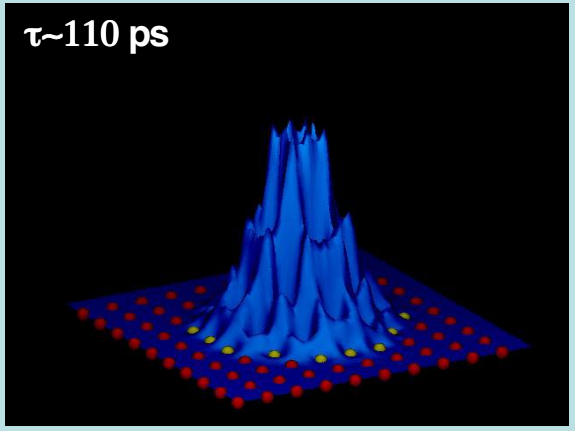


Delocalized positron density

Vacancy defects



Embedded particles of stronger positron affinity

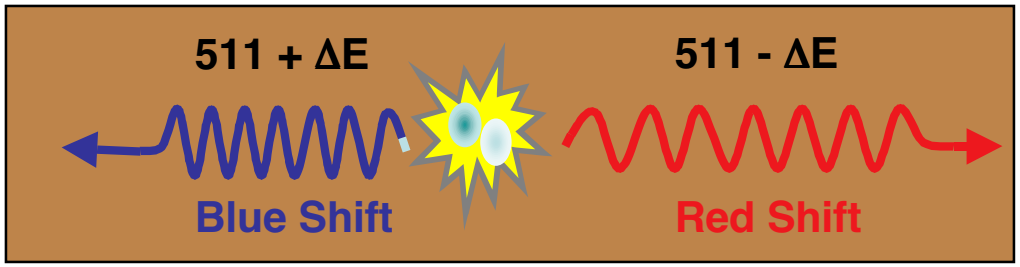


Strongly localized positron density

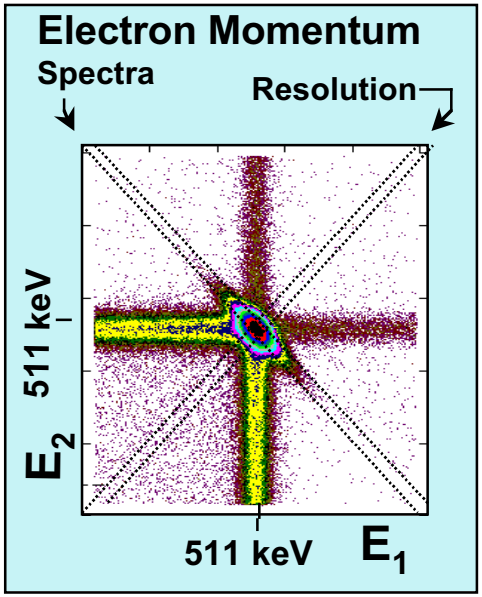
Each defect has a characteristic positron lifetime, τ, determined by the overlap of electron and positron charge densities

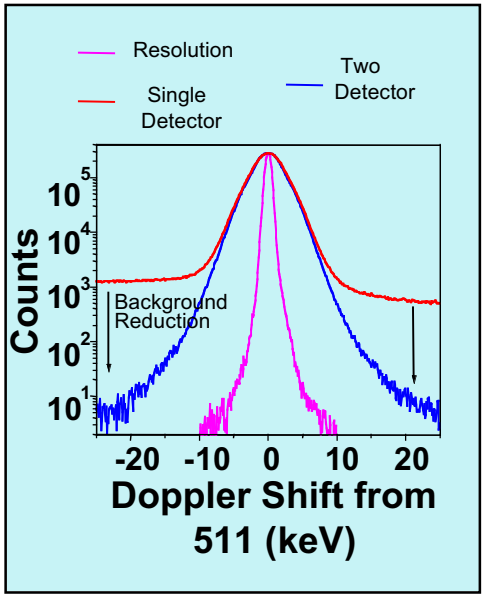
Doppler broadening of annihilation photons

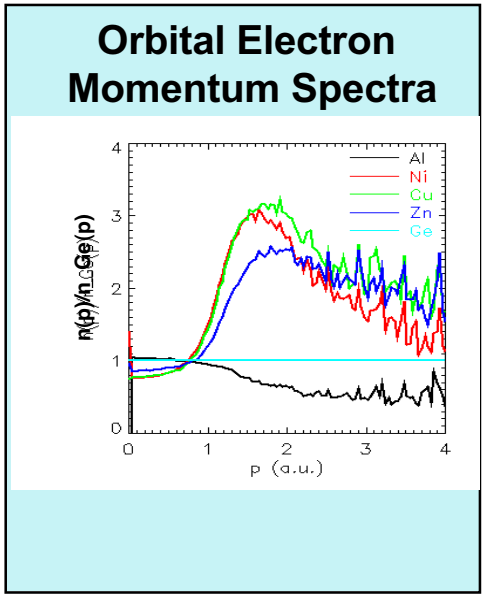
Doppler shift probes the local electron momentum



Doppler shift, ΔE Is proportional to electron momentum, p_L







Coincident, two - detector spectroscopy improves signal-to-noise ratio

Kinematic cuts provide momentum spectra of orbital electrons
Orbital electron momentum spectra (OEMS) are element-specific

Modeling predictions & positron theory

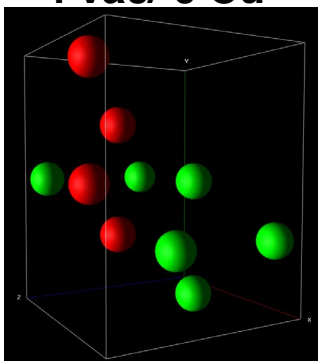
Kinetic Monte Carlo modeling predicts formation of a continuum of vacancy-solute (Cu) cluster complexes

KMC predictions

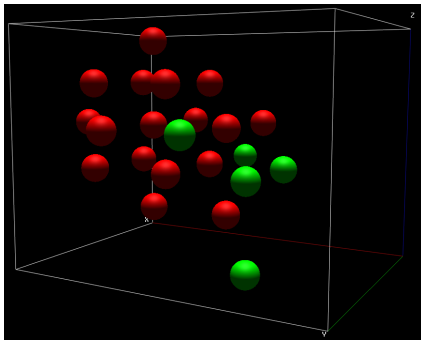
vac

Cu

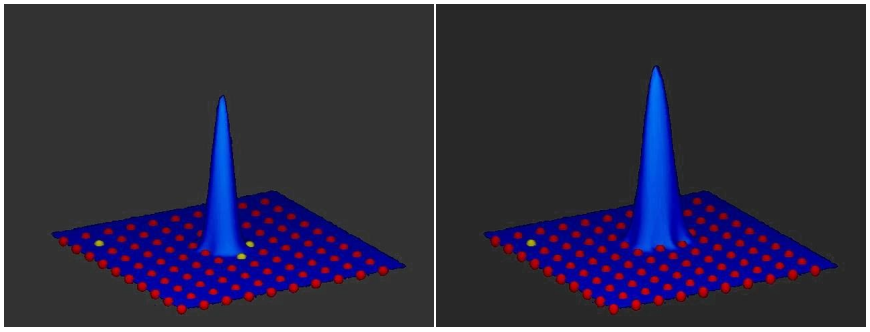
4 vac/ 6 Cu



17 vac/ 5 Cu



Calculated positron density



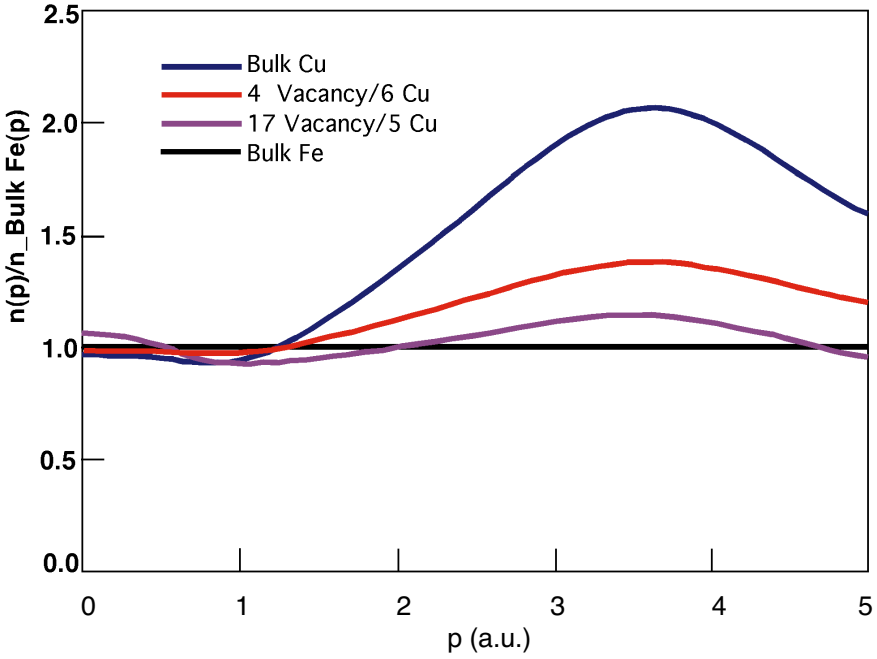
Calculated positron lifetime

216 ps

350 ps

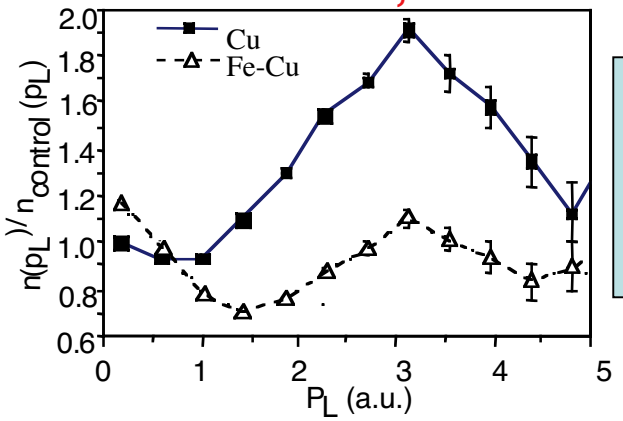
Modeling predictions & positron theory

Calculated positron OEMS



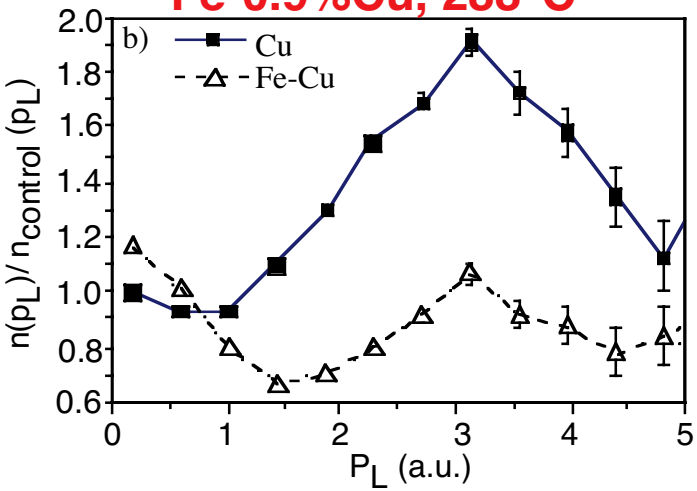
Vac/Cu	τ (ps)
3/6	173
4/6	216
17/5	350
>50/x	520

Fe-0.9%Cu, 60°C



τ (ps)
178
355

Fe-0.9%Cu, 288°C



τ (ps)
222
520