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Comparison of MD and BCA for Displacement Cascades in GaAs

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Comparison of MD and BCA Methodologies

	Binary Collision Approx. (Marlowe)	Molecular Dynamics
Interatomic Interactions	Short-range repulsion (ZBL)	Cohesive model based on covalent bonding plus short-range repulsion (ZBL)
Dynamics	Series of binary collisions	Fully-coupled atomic dynamics
Threshold Displacement Energy	*Adjustable parameter*	Predicted (9 eV)
Electronic Stopping	ZBL model	Lindhard-Scharf
Nature of output data	Location of point defects – only type of damage model can predict	Atomic positions – analysis produces point defects and amorphous zones
Combination of near defects	Adjacent defects combined if appropriate	Adjacent defects combined if appropriate

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MD simulation details

- **Analytic Bond Order Potential (BOP) for GaAs interatomic potential**
  - Short-range behavior corrected to match standard 'ZBL' short-range ionic repulsion
- **LAMMPS MD code**
  - Widely-used internationally
- **Simulation Setup**
  - Periodic Boundary Conditions
    - 64,000 atoms for 100 eV; 13,824,000 atoms for 50 keV
  - Mixed 'NVE' and Langevin simulations
    - Standard NVE dynamics in the center of cell
    - Langevin random forces added around edge of cell
  - Simple treatment of electronic stopping through a velocity dependent drag term
    - Lindhard-Scharff model
  - Dynamic time step adjustment

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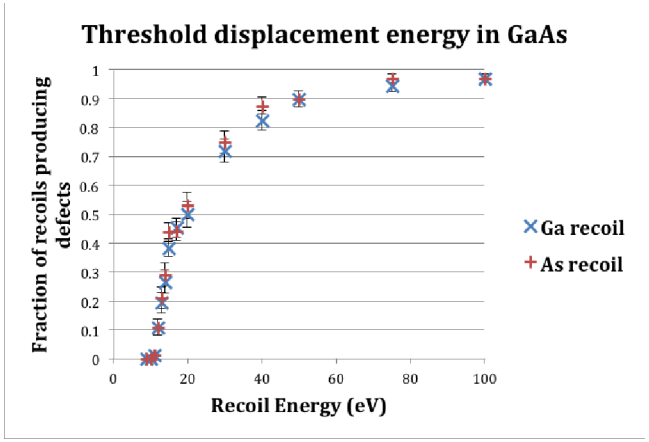
BOP *predicts* reasonable threshold displacement energies

- **Experimental information based on electron irradiation**
  - **Threshold energy on the As sublattice: 9-10 eV**
  - **Threshold energy on the Ga sublattice: undetermined**
    - **Cannot observe these defects even at cryogenic temperatures**
    - **Pons and Bourgoin, J of Phys C: Solid State Physics 18, 3839 (1985)**
- **BOP simulation results are *predictions***
  - ***Validation* data point**



- **MD predicted threshold energy**
  - **11 eV**
- **Recoil direction at threshold**
  - **<1 1 1> - along nearest neighbors**

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A combination of analysis algorithms is used to identify defects

- **Analysis of ring structures to define non-crystalline regions**
  - **Ring is a closed path of nearest neighbor hops**
    - **For ideal diamond structure, shortest non-trivial rings are 6- and 8-member paths**
    - **Amorphous structures have significant numbers of 5- and 7-member rings**
  - **Local high density of 5- and 7-member rings will be taken to mean locally non-crystalline (amorphous) material**
- **For regions which are "crystalline" by the above criterion, use a cell method based on an ideal lattice to define defects**
  - **Examine occupation of cell around each ideal lattice sites**
  - **Defects are defined by deviations from ideal occupation**
    - **Vacancy: empty cell**
    - **Interstitial: multiply occupied cell**
    - **Anti-site defect: atom of wrong type in cell**

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Assume recombination of defects on nearest neighbor sites

- Analogous to combination of defects in Marlowe
- Combinations occur between nearest neighbor sites
  - Vacancy and interstitial
    - Same types -> annihilate
    - Opposite types -> anti-site defect
  - Vacancy and an anti-site
    - ‘a’ vacancy + a(b) anti-site -> ‘b’ vacancy
  - Interstitial and an anti-site
    - ‘a’ interstitial + b(a) anti-site -> ‘b’ interstitial
  - Repeat these combinations until a ‘stable’ state is reached

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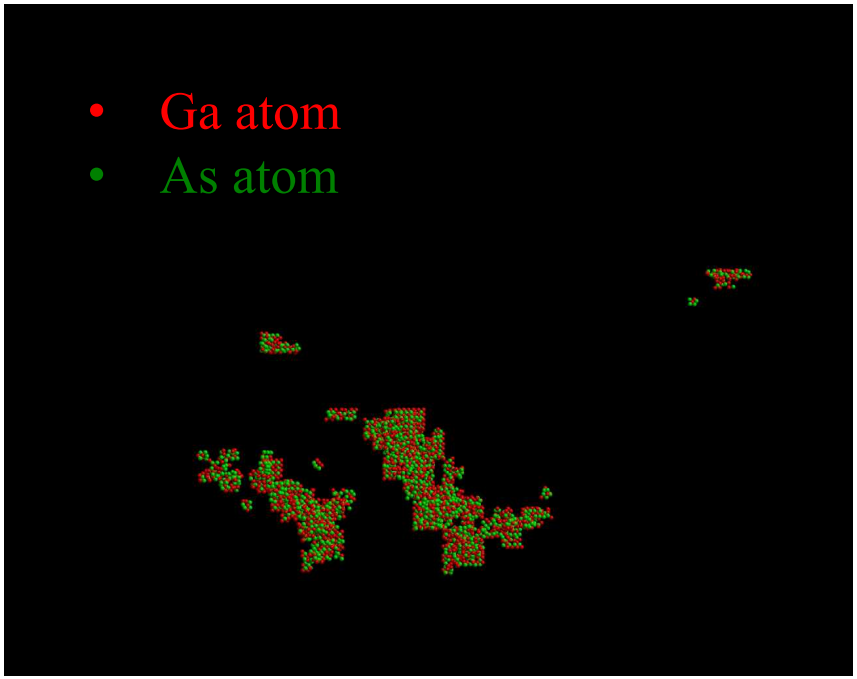
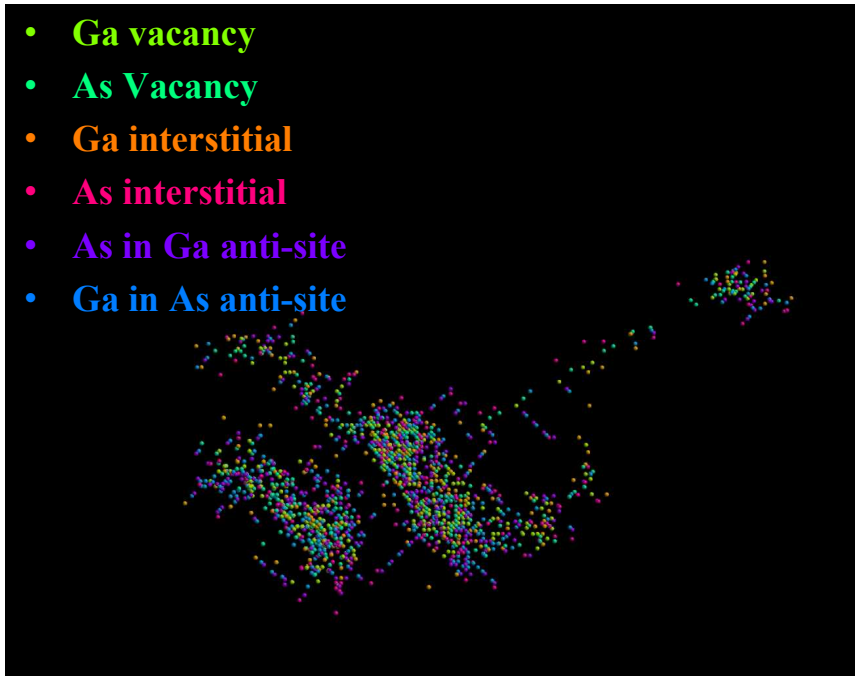
Example of Defect Identification 50 keV recoil in GaAs

Amorphous zones



- Breaks into subcascades
- Electrical Consequences?

Point Defects



- Point defects are highly clustered
  - Related to lack of lack of well-defined states in DLTS?

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BCA assumes an "Effective Threshold Displacement Energy"

- ***Effective*** **Threshold energy is one of the key physical input parameters for a BCA calculation**
  - **In collision sequence, if a recoil energy is less than the threshold, ion is assumed to stay in its lattice site**
  - **Effective threshold energy has a strong influence on the predicted number of defects**
- **Effective threshold for BCA is *NOT* the experimentally determined threshold displacement energy**
  - **Threshold displacement energy is a lower bound**

What insight can MD give on the choice of the BCA Effective Threshold Energy?

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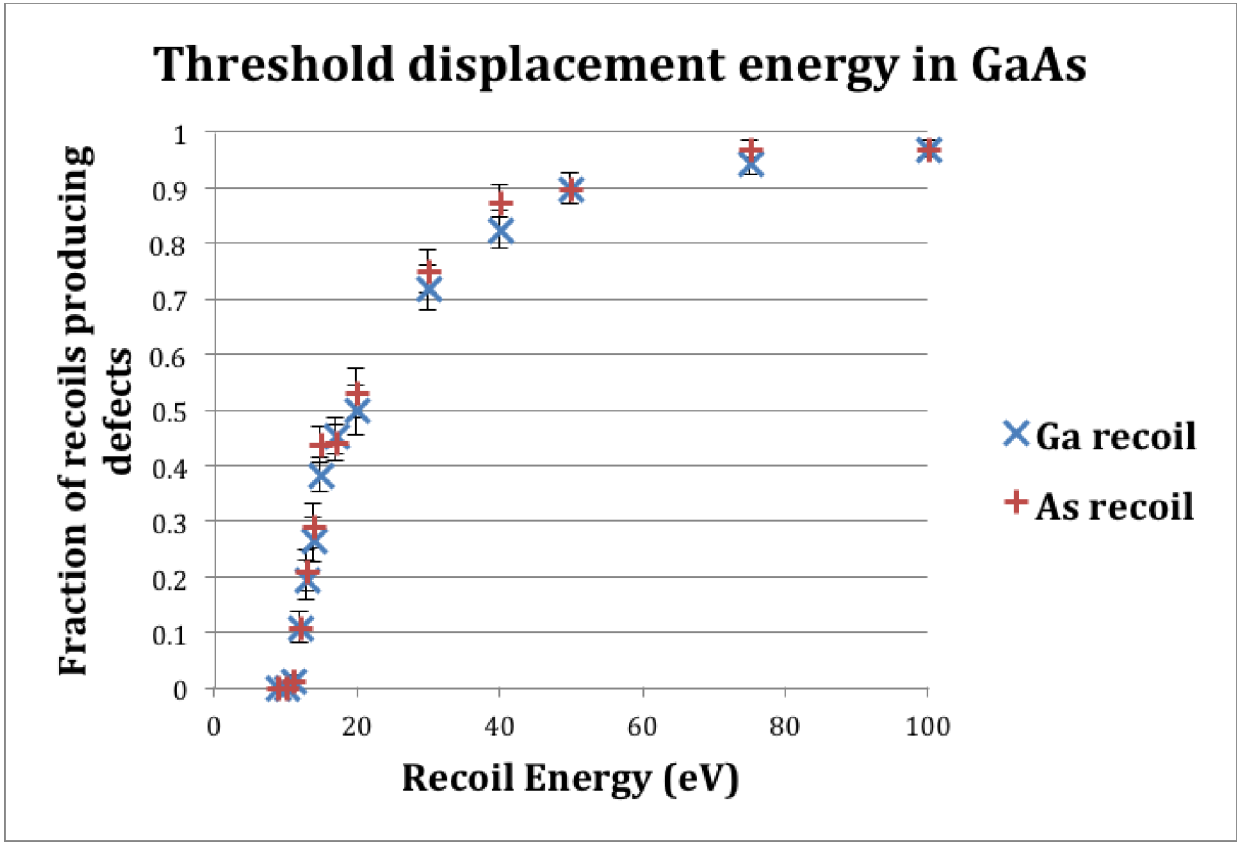
MD determines probability of defect production



- MD simulations of recoils for varying energies – at each energy a uniform grid of recoil directions was simulated

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First MD estimate of effective threshold energy

- There is not a rigorous way to relate the recoil probability to the effective energy
  - Various approaches in the literature
- Simple, intuitively appealing criteria
  - Effective threshold energy is the energy where there is a 50% chance of persistent damage
    - 19 eV
  - Since MD overestimates the experimental threshold by 2 eV, should adjust this estimate to 17 eV

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Second approach for effective threshold Compare predicted number of defects

- MD simulations yield a predicted number of defects at selected energies
  - Consider 10 keV and 50 keV recoils
  - 10 MD runs at each recoil energy and species
- BCA calculations were performed at the same recoil energies with a range of assumed effective threshold energies
  - 500 runs at each set of conditions

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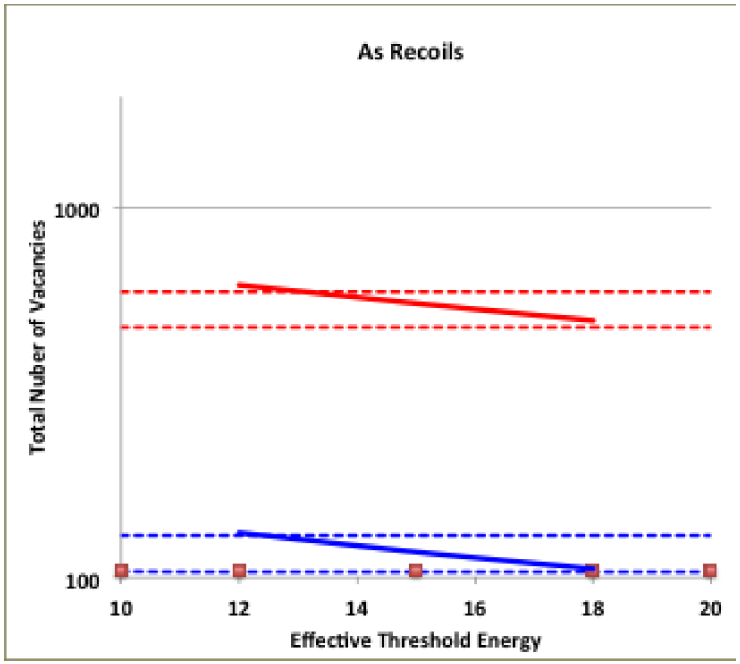
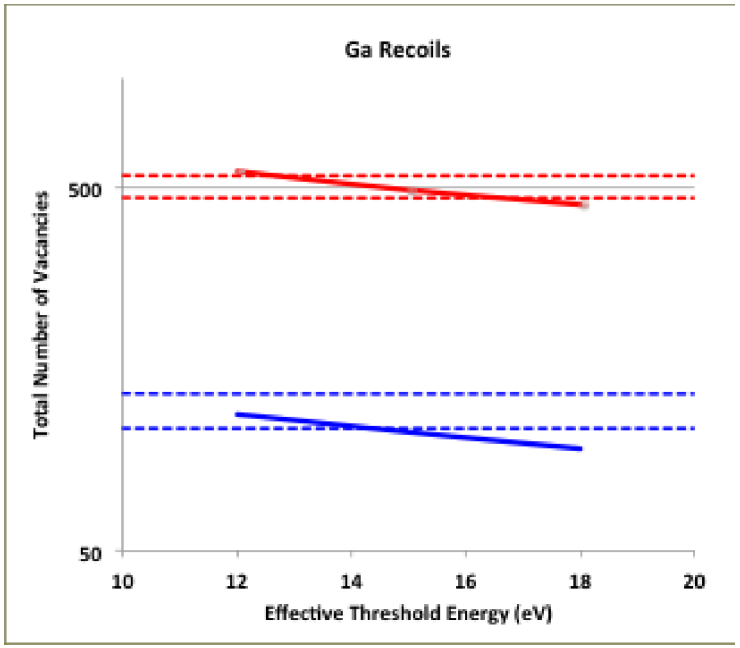
Comparison of vacancy production for different effective threshold energies





- **Red – 50 keV recoils; Blue – 10 keV recoils**
  - **Solid lines – BCA data**
  - **Dotted lines – range of MD results**
- **Effective threshold of about 15 eV is consistent with this data.**

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Comparison of the predicted defect number MD vs BCA

Recoil Type	Defect	MD 10 keV	BCA 10keV	MD 50 keV	BCA 50 keV
Ga	Ga int.	44.2 ± 1.8	52.9 ± 0.5	188.9 ± 9.6	248.2 ± 2.9
As	Ga int.	46.3 ± 2.9	58.3 ± 0.5	194.7 ± 10.3	277.8 ± 2.7
Ga	As int.	45.7 ± 4.7	50.9 ± 0.5	196.8 ± 11.2	240.1 ± 2.9
As	As int.	41.1 ± 4.3	57.4 ± 0.5	203.2 ± 11.2	271.8 ± 2.6
Ga	Ga anti-site	76.1 ± 6.4	21.8 ± 0.3	329.1 ± 18.5	102.0 ± 1.4
As	Ga anti-site	68.4 ± 5.7	23.4 ± 0.3	349.2 ± 15.0	118.8 ± 1.5
Ga	As anti-site	75.7 ± 6.0	22.7 ± 0.3	319.7 ± 19.9	109.0 ± 1.5
As	As anti-site	69.5 ± 7.0	24.3 ± 0.3	346.4 ± 15.6	124.6 ± 1.6

- **Use BCA effective threshold of 15 eV**
- **Resonable agreement for interstitials**
- **Serious discrepancy on the number of anti-site defects**

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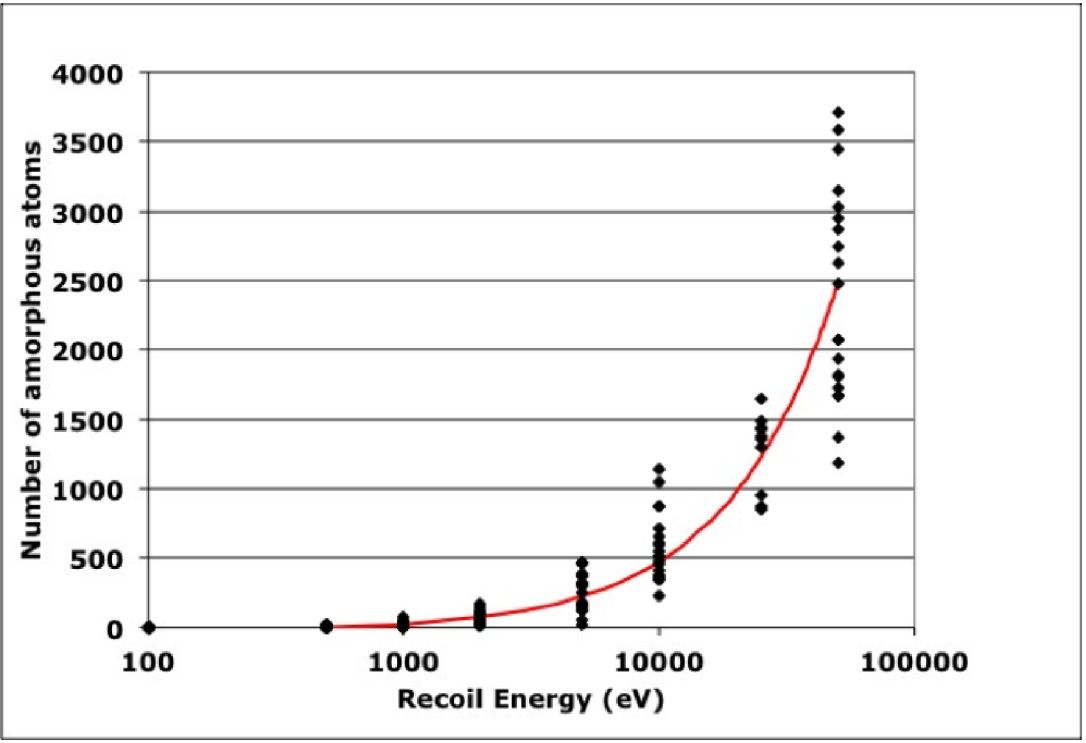
There is a threshold energy for the production of amorphous regions



- Threshold for production of amorphous GaAs between 500 and 1000 eV
  - Similar threshold observed for Si between 200 and 500 eV
    - Srour notes the onset of "clustered defects" in Si at 400 eV
- Number of amorphous atoms increases roughly linearly above this threshold
  - Slope ~ 0.05/eV

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Coordination of amorphous atoms MD and Expt in agreement

- **Experimental estimate of the average coordination**
  - **3.85±0.20**
  - **M.C. Ridgway, NIMPR B 148. 391 (1999)**
- **MD prediction**
  - **3.9**

- **Validation point for the MD simulations**

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Most amorphous atoms do NOT have ideally coordinated environment

		Number of Neighbors of Same Species				
		0	1	2	3	4
Total Coordi-nation	2	0.013	0.008	0.000		
	3	0.056	0.054	0.032	0.006	
	4	0.268	0.281	0.115	0.024	0.002
	5	0.010	0.061	0.046	0.014	0.001

- 69% of atoms are four-fold coordinated
  - 15% are 3-fold coordinated
  - 13% are 5-fold coordinated
- Only 27% of atoms have ideal coordination including composition
  - Compositional defects are common

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Future Direction: Electronic Properties of Amorphous Zones

- **Small candidate amorphous structures will be generated for DFT studies**
  - Cell need to to 500 – 1000 atoms
  - Cut out of MD simulations or generated to agree with MD structural data
- **DFT simulations will be performed using QUEST**
  - Are there states deep in the gap that could be candidates sources of the U-band?
  - Are amorphous zones charged?
- **Initial Goal: Decide if the amorphous zones deserve further examination**

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BACKUP SLIDES

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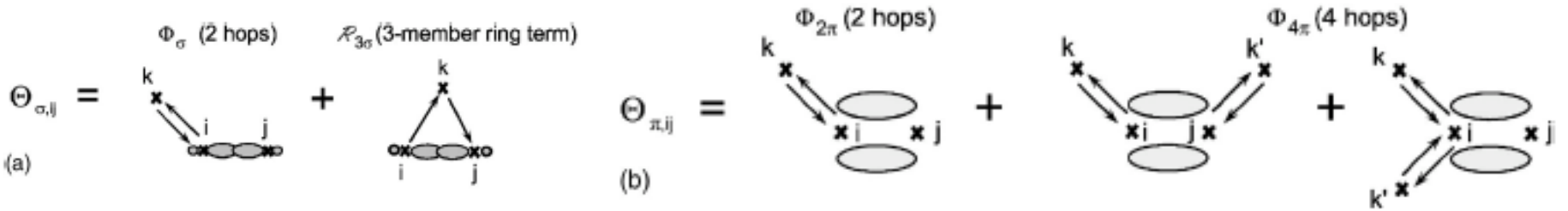
"Bond Order Potentials" (BOP) provide a physically-based interaction model

- **Advantages**
  - Derived from a tight-binding description of covalent bonding
    - Approximates the quantum mechanical basis of bond formation
  - A parameterization exists for GaAs
    - Murdick, Zhou, Wadley, Nguyen-Manh, Drautz and Pettifor, Phys. Rev. B 73, 045206 (2006)
  - Structural and binding energy trends generally match experiment and ab initio calculations
- **Disadvantages**
  - Computational expense at least an order of magnitude higher than Tersoff-style potentials used for Si studies
  - Less accurate than electronic structure calculations (DFT)



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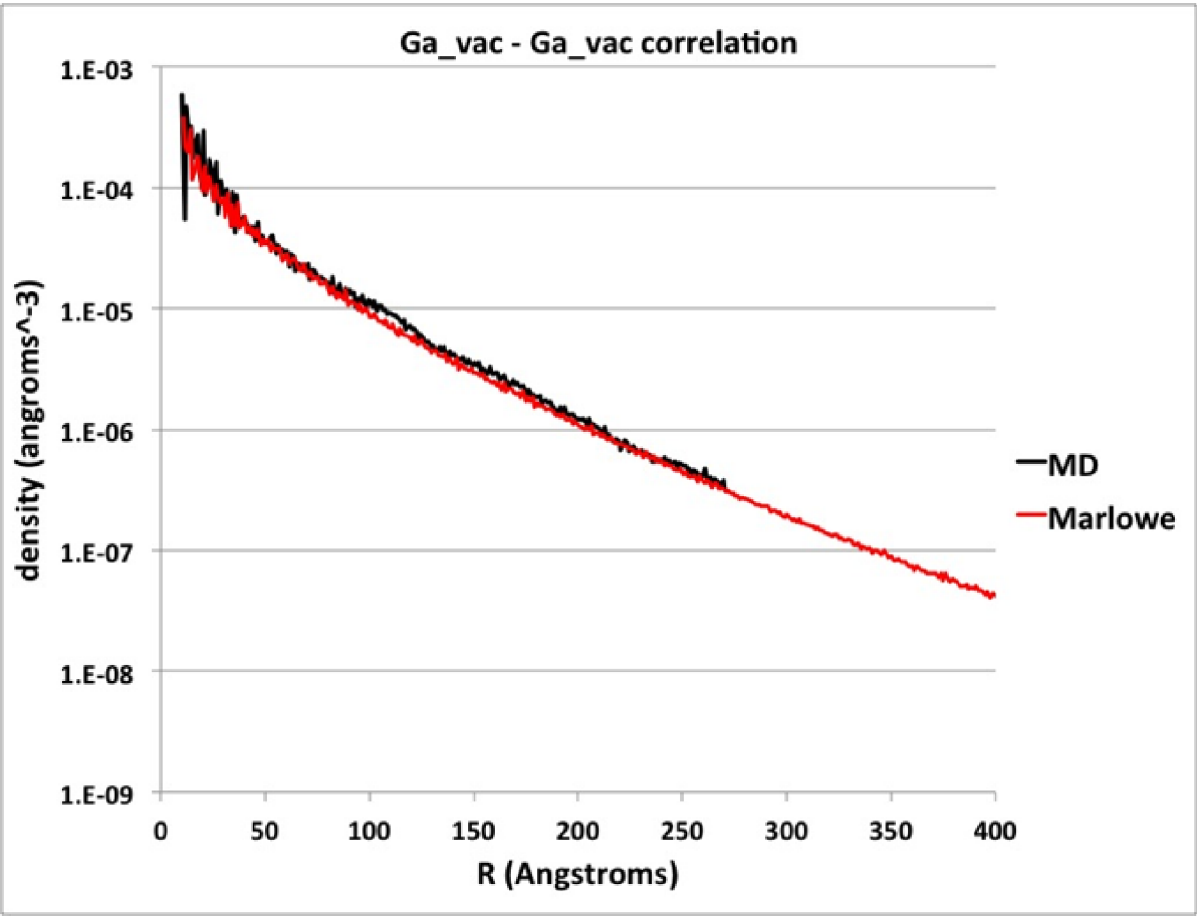
Sample correlation comparison Ga_vacancy – Ga_vacancy



- **BCA and MD predict very similar defect clustering!**
- **Level of agreement similar for other defect combinations except for overall offset due to different number of defects**

50 keV Ga recoils

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