SAND2009-4715C

Molecular Dynamics Simulations of Displacement Cascades in GaAs

Stephen M. Foiles
Computational Materials Science and Engineering Dept.
Sandia National Laboratories
Albuquerque, NM, USA

Presented at
Session 2: Computational Methods and Radiation Effects
Joint U.S. Russia Conference on Advances in Materials Science
August 30 – September 3, 2009
Prague, Czech Republic

NNSA National Nuclear Security Administration

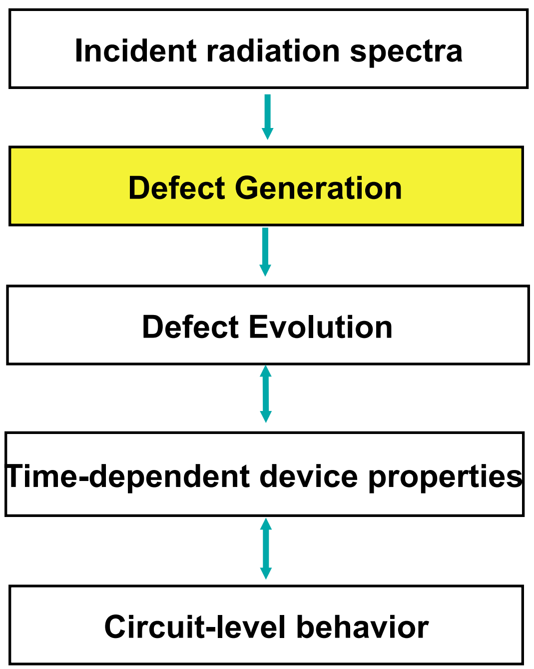
Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration, under contract DE-AC0494AL85000.

Sandia National Laboratories

Sandia is quantifying the impact of neutron exposure on performance of GaAs-based electronics

Modeling goal: physics-based description of the time-dependent properties of *irradiated* transistors and their circuits

Phenomena required in the model

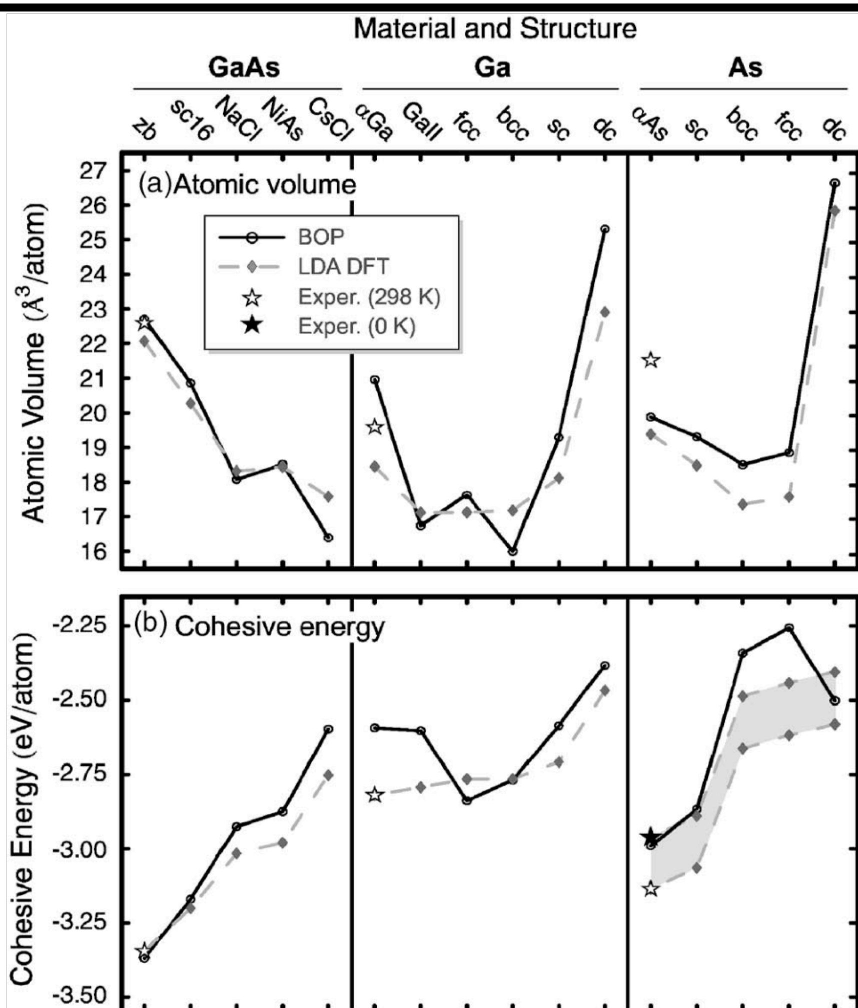


- Require predictions of the number and type of defects produced by the incident radiation for subsequent device level models
- Molecular dynamics (MD) is being pursued to provide support for binary collision approximations (BCA) calculations of defect generation
  - Number of defects produced
  - Spatial distribution of defects produced
  - Initial correlations among the defect species
  - Amorphous zones

“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
    - Examples to follow
- Disadvantages
  - Computational expense at least an order of magnitude higher than Tersoff -style potentials
    - Complex force evaluations
  - Until recently, only a serial implementation available
    - Limited initial calculations to a few hundred atoms
    - Have completed massively parallel implementation in the LAMMPS MD code

BOP predictions of structural trends in reasonable agreement with *ab initio* results



Murdick, Zhou, Wadley, Nguyen-Manh, Drautz and Pettifor, Phys. Rev. B 73, 045206 (2006)

- Reproduces trends in energies with variations in structure
  - Gives confidence in transferability of results to defected structures

BOP predictions for point defects in reasonable accord with *ab initio* calculations

	DFT[a]			BOP		
Defect	E'_D	$\hat{r}_{NN}$	Type(No.)	E'_D	$\hat{r}_{NN}$	Type(No.)
V_{Ga}	3.15	0.88	As(4)	3.28	0.99	As(4)
V_{As}	3.10	0.89	Ga(4)	2.93	1.03	Ga(4)
Ga_{As}	2.12	0.99±0.06	Ga(4)	2.03	1.06	Ga(4)
As_{Ga}	2.48	1.06	As(4)	2.50	1.05	As(4)
Ga_i (tetrahedral)	2.98	1.06	As(4)	2.66	1.03	Ga(4)
				4.14	1.08	As(4)
As_i (tetrahedral)	5.04	-	Ga(4)	4.47	1.07	Ga(4)
				3.32	1.03	As(4)
Ga_i ($\langle 110\rangle$ dumbbell)	3.53	-	Ga(1)/As(3)	4.97	1.01/1.01–1.02	Ga(1)/As(3)
As_i ($\langle 110\rangle$ dumbbell)	4.07	1.01/1.07	As(1)/Ga(3)	3.82	0.94/1.02–1.08	As(1)/Ga(3)
Ga_i ($\langle 100\rangle$ dumbbell)	-	-	-	3.86	0.89/0.96	Ga(1)/As(2)
As_i ($\langle 100\rangle$ dumbbell)	-	-	-	4.68	0.88/0.99	As(1)/Ga(2)

Murdick, Zhou, Wadley, Nguyen-Manh, Drautz and Pettifor, Phys. Rev. B 73, 045206 (2006)

- Better representation of point defect energies than other competing potentials
- Issues with the As interstitial

QASPR
QUALIFICATION ALTERNATIVES TO SPR

Sandia National Laboratories

MD simulation details

- Analytic Bond Order Potential for GaAs interatomic potential
  - Murdick, *et al.*, Phys. Rev. B 73, 045206 (2006)
- Short-range behavior corrected to match models of short-range ionic repulsion
  - 'ZBL'
    - J.F. Ziegler, J.P. Biersack and U. Littmark, The Stopping and Range of Ions in Solids, 1985
    - Fit to electronic structure calculations of ionic repulsion for a range of ionic pairs
- LAMMPS parallel MD code
  - New implementation of the BOP interatomic potential
- 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 - Phys. Rev 124, 128 (1961)
  - Dynamic time step adjustment
    - Time step chosen such that dr < 0.001 Å in a given step

QASPR QUALIFICATION ALTERNATIVES TO SPR

Sandia National Laboratories

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
- For defects on nearest neighbor sites, perform simple recombinations where appropriate
  - For example, adjacent vacancy and interstitial defects combine to either annihilate or create an anti-site defect

BOP predicts reasonable threshold displacement energies

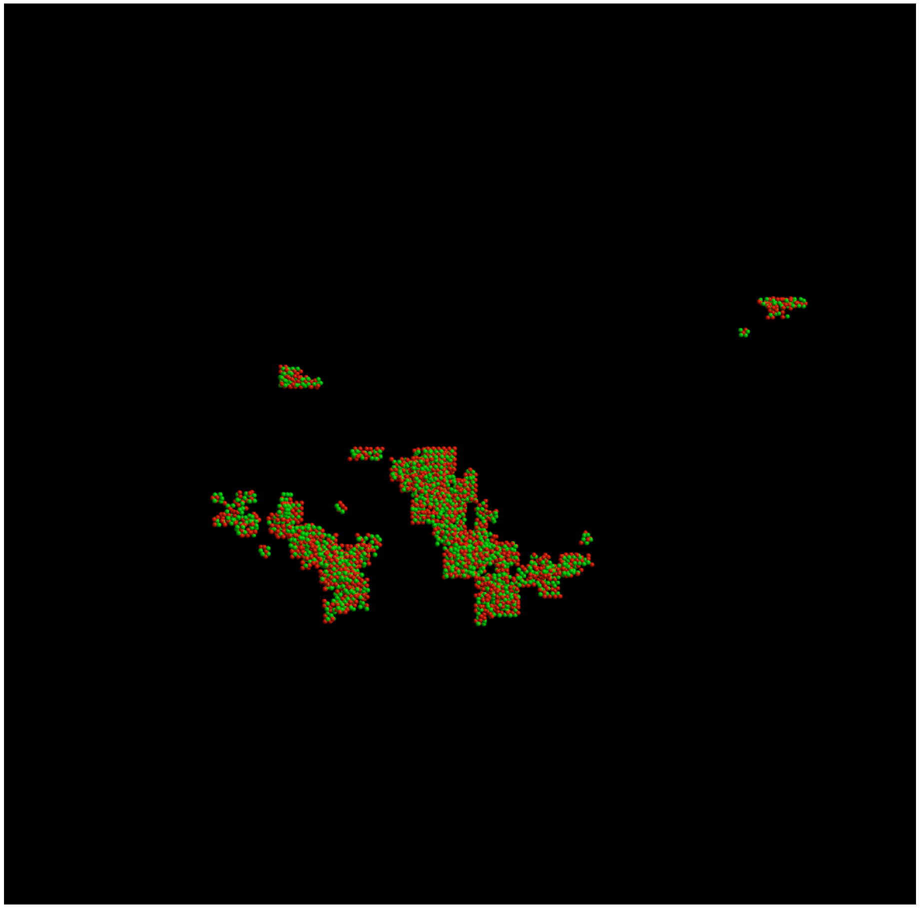
- MD simulations of low-energy recoils using BOP
  - Threshold energy on Ga sublattice: ~9 eV
  - Threshold energy on As sublattice: ~12 eV
- Experimental information based on electron irradiation
  - Threshold energy on the As sublattice: 9-10 eV
    - Sublattice determined by examination of dependence of defect formation on the crystal orientation of electron irradiation
  - Threshold energy on the Ga sublattice: undetermined
    - Frenkel pairs on the Ga sublattice are assumed to have very short lives due to the opposite charge of the Ga vacancy and interstitial
    - 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*
- Previous Tersoff-style interaction models either
  - Poor point defect predictions
  - Poor threshold displacement energy predictions

QASPR QUALIFICATION ALTERNATIVES TO SPR

Sandia National Laboratories

Amorphous Region in 50 keV recoil in GaAs

- Red: Amorphous Ga
- Green: Amorphous As
- Amorphous regions
  - Are of significant size
  - Break into subcascades



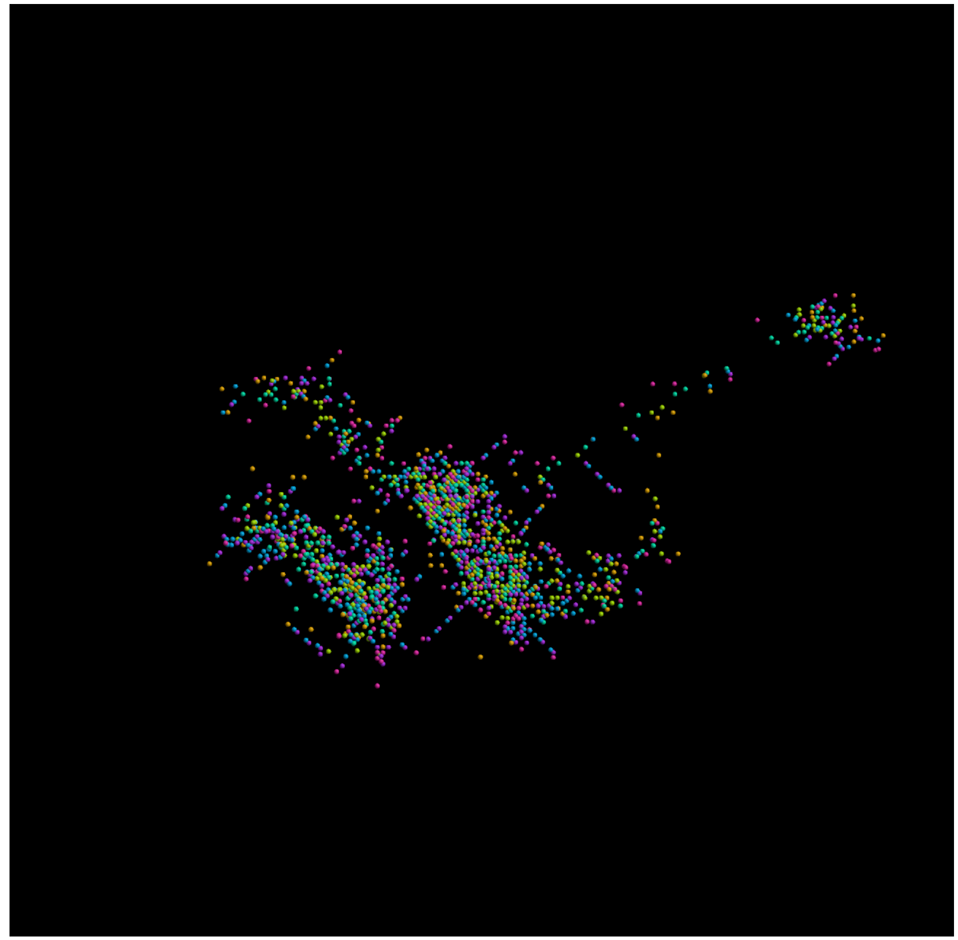
50 nm

QASPR QUALIFICATION ALTERNATIVES TO SPR

Sandia National Laboratories

Point Defects produced by a 50 keV recoil in GaAs

- Most of the point defects cluster into sub-cascades
  - Around amorphous zones
- Degree of clustering suggests that one cannot treat this as a collection of isolated point defects
  - Need to consider point defect correlations
  - Consistent with the absence of well defined electronic states in experiments such as Deep-Level -Transient-Spectroscopy (DLTS)
- Visual inspection shows a large number of Anti-site defect pairs



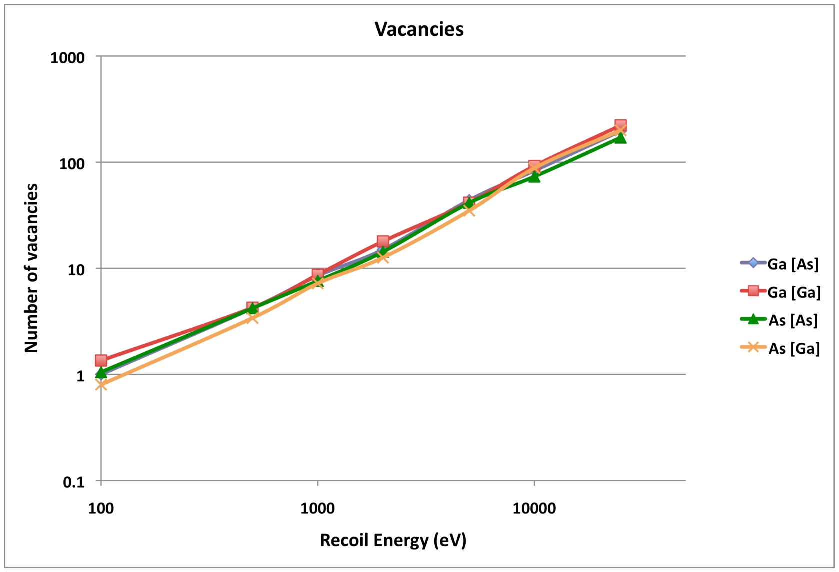
50 nm

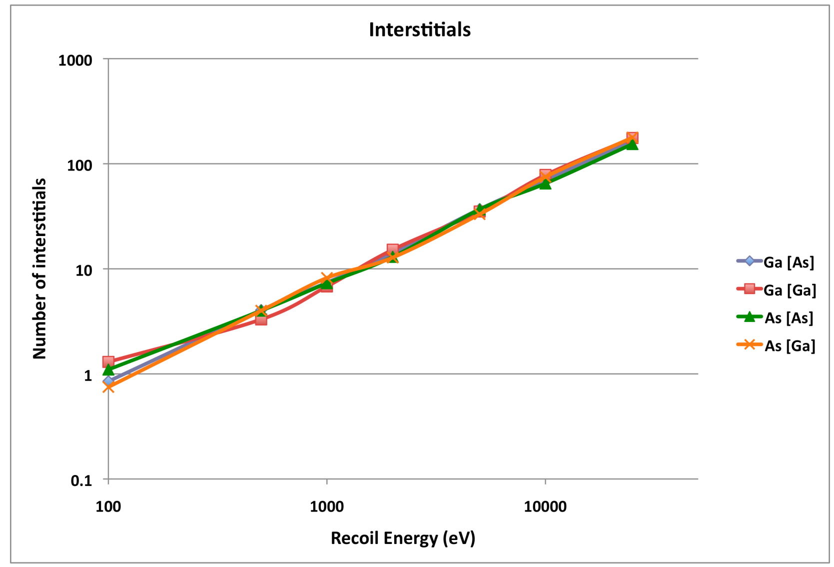
- Ga vacancy
- As Vacancy
- Ga interstitial
- As interstitial
- As in Ga anti-site
- Ga in As anti-site

QASPR
QUALIFICATION ALTERNATIVES TO SPR

Sandia National Laboratories

Quantification of the production of Vacancies and Interstitials



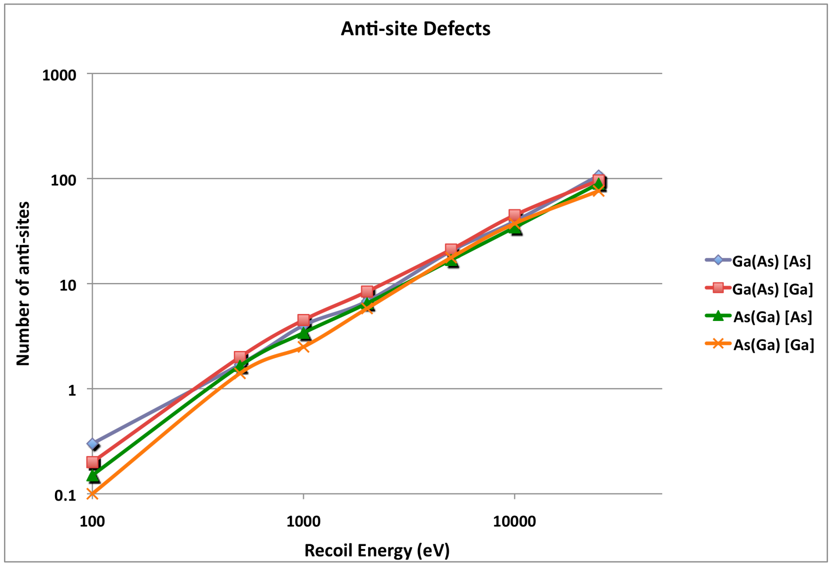


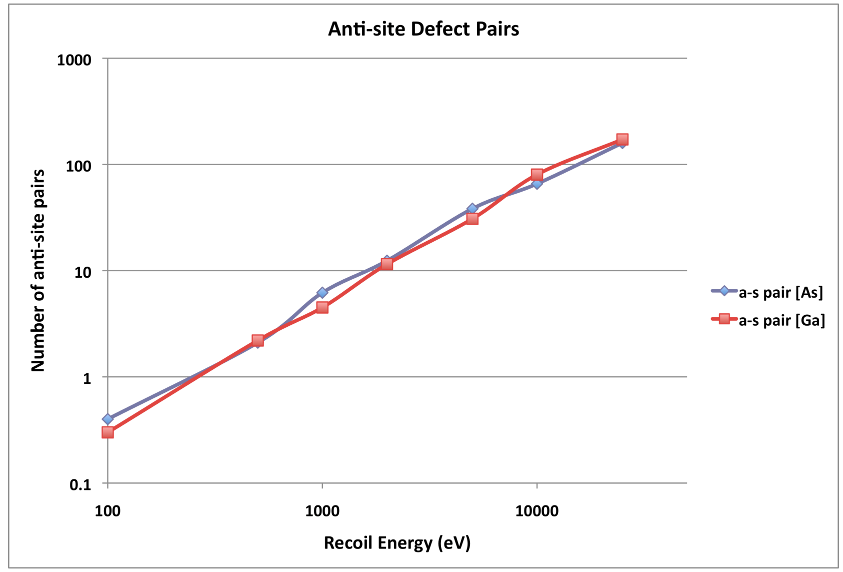
- The number of vacancies and interstitials increases roughly linearly with recoil energy for the range of energies considered.
- There is NOT is significant difference between
  - Defects produced on either the Ga or As sublattice.
  - Chemical identity of the initial primary knock-on atom (PKA)

QASPR
QUALIFICATION ALTERNATIVES TO SPR

Sandia National Laboratories

Large number of anti-sites defects generated
Anti-sites often occur in pairs



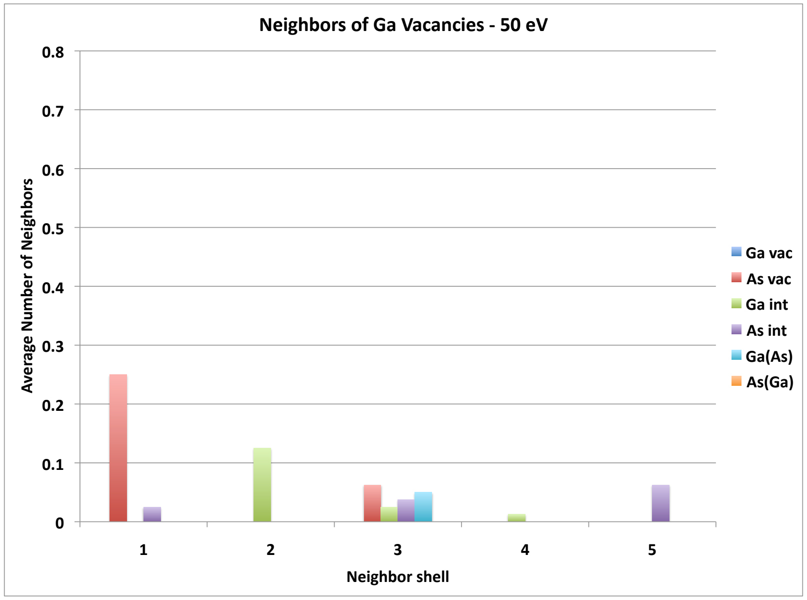


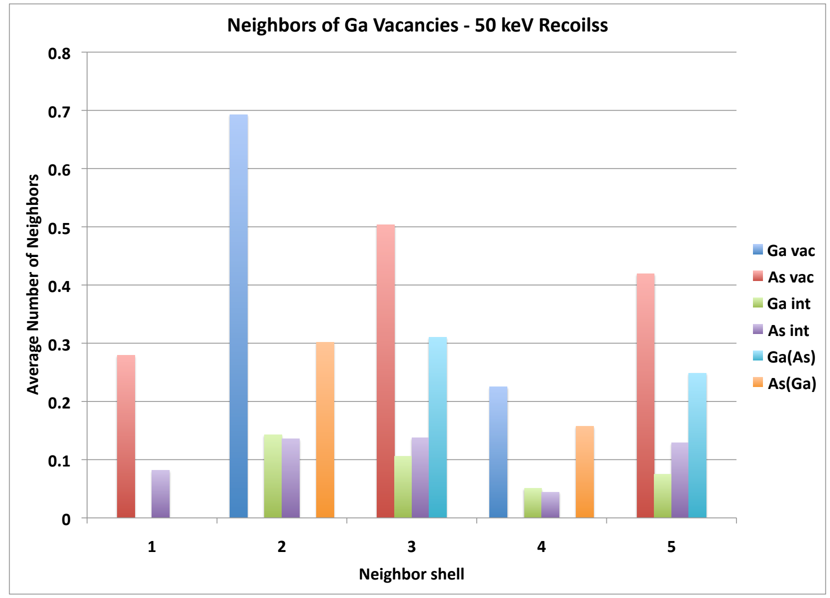
- The number of isolated anti-site defects is comparable to the number of vacancies or interstitials
- Many of the anti-site defects occur in nearest neighbor pairs of the opposite sign
  - Could result from replacement sequences

QASPR
QUALIFICATION ALTERNATIVES TO SPR

Sandia National Laboratories

Example of correlations of point defects
Ga vacancy





- About a quarter of the Ga vacancies have a As vacancy in the first neighbor shell at all the energies studied
  - Similar to the observation in Si that there are many initial di-vacancies
- At higher energies, there are numerous Ga vacancies in the second neighbor shell

QASPR QUALIFICATION ALTERNATIVES TO SPR

Sandia National Laboratories

Summary and Future Work

- Performed MD simulations of displacement cascades in GaAs
  - Implemented BOP interatomic potential for GaAs
  - Identify amorphous regions in cascade and point defects in the approximately crystalline regions
- Quantified the number of defects produced as a function of recoil energy
  - Results will be compared to predictions of simpler binary collision approximation (BCA) simulations
- Observed strong clustering of the defects produced
  - Higher scale models will need to consider this clustering in continuum level descriptions of the defect evolution
  - Will explore the relationship between this clustering and experimental studies, such as DLTS, of the electronic properties of irradiated GaAs