Computational Modeling of Amorphous Materials

Brittany Hoard

Advisor: Dr. Blair Tuttle

Penn State Erie, The Behrend College

Outline

- Intro
- Amorphous Si
  - Goal: Determine point defects in solar cells
- Interfaces with amorphous materials
  - Goal: Structure of interface

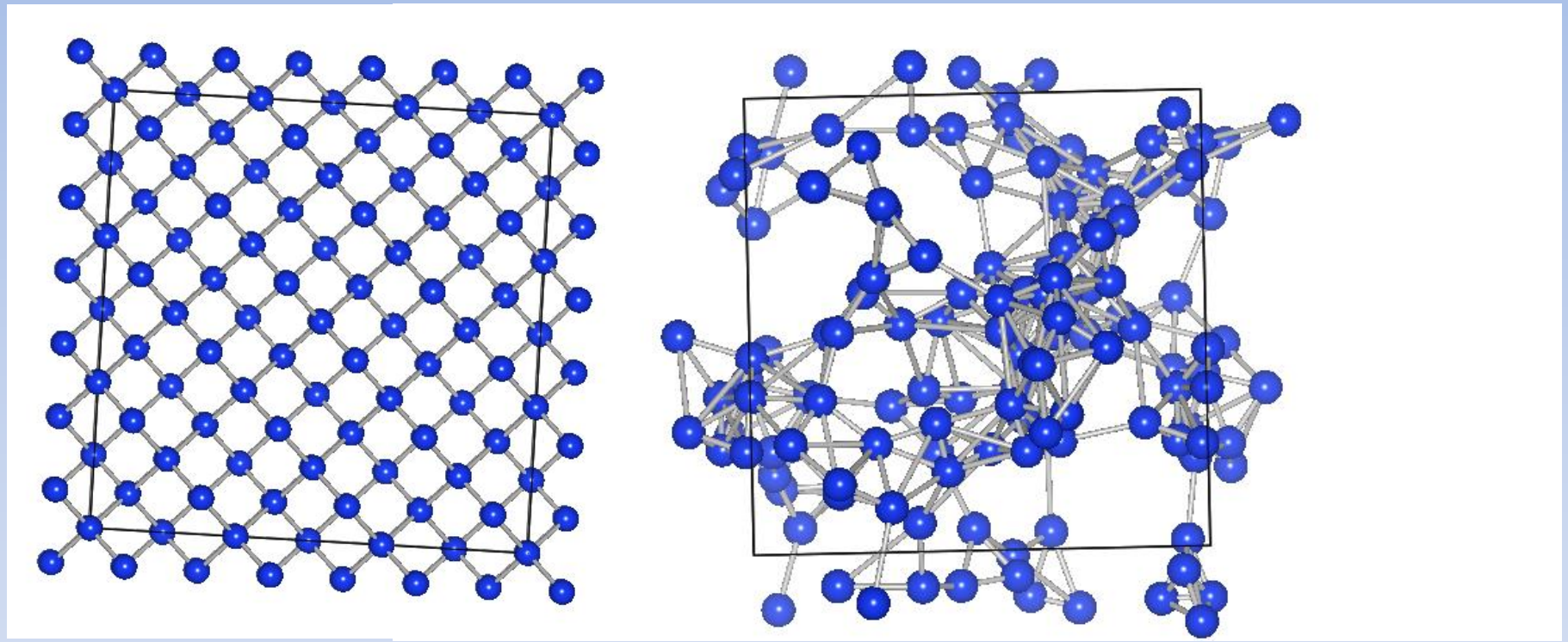
Introduction

- Atomic structure of amorphous materials
- Wooten, Winer, and Weaire (WWW) algorithm
- Behrend Amorphous Modelling (BAM) code
  - Research, education
- Amorphous silicon (a-Si)
  - Semiconductor, solar cells
- Amorphous Interfaces
  - electronics

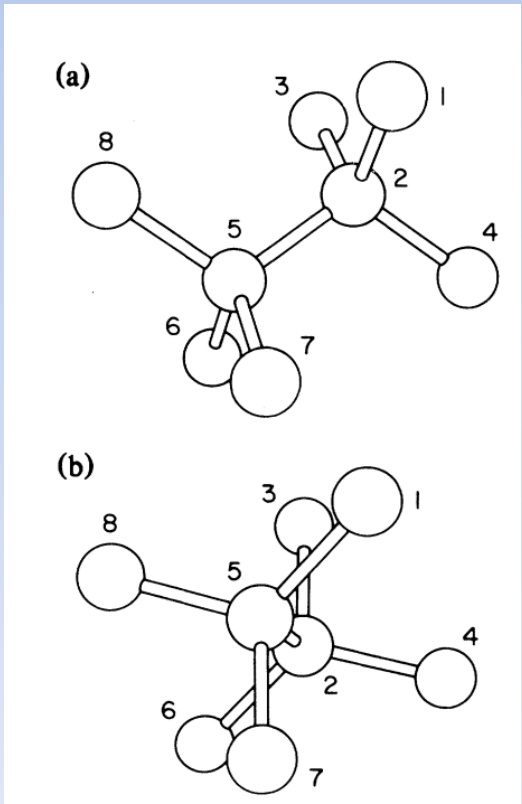
Amorphous Si

- Create low energy amorphous model
- Create models with defects
- Study electronic properties of defects in models

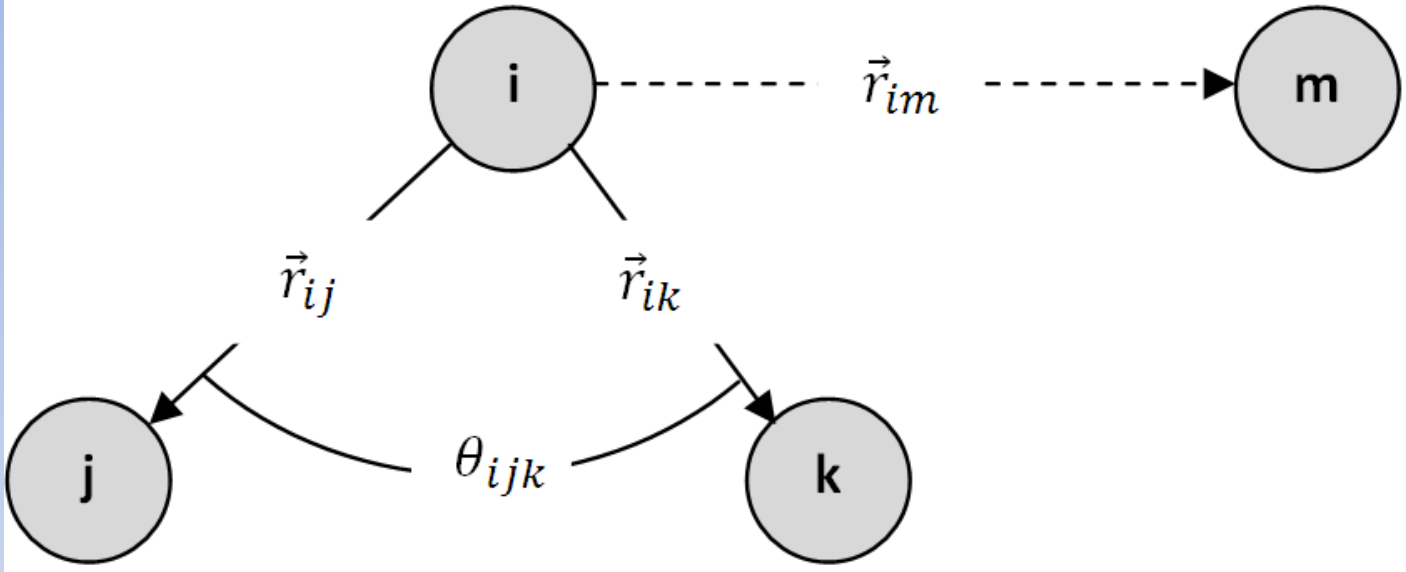
Starting Structure



Bond swapping



Energy: Keating Potential



$$PE_{radial} = \frac{1}{2}\sum_{i\in\alpha}\sum_{j\in\beta_i}\frac{1}{2}k_r\left(\|\vec{r}_{ij}\| - r_0\right)^2$$

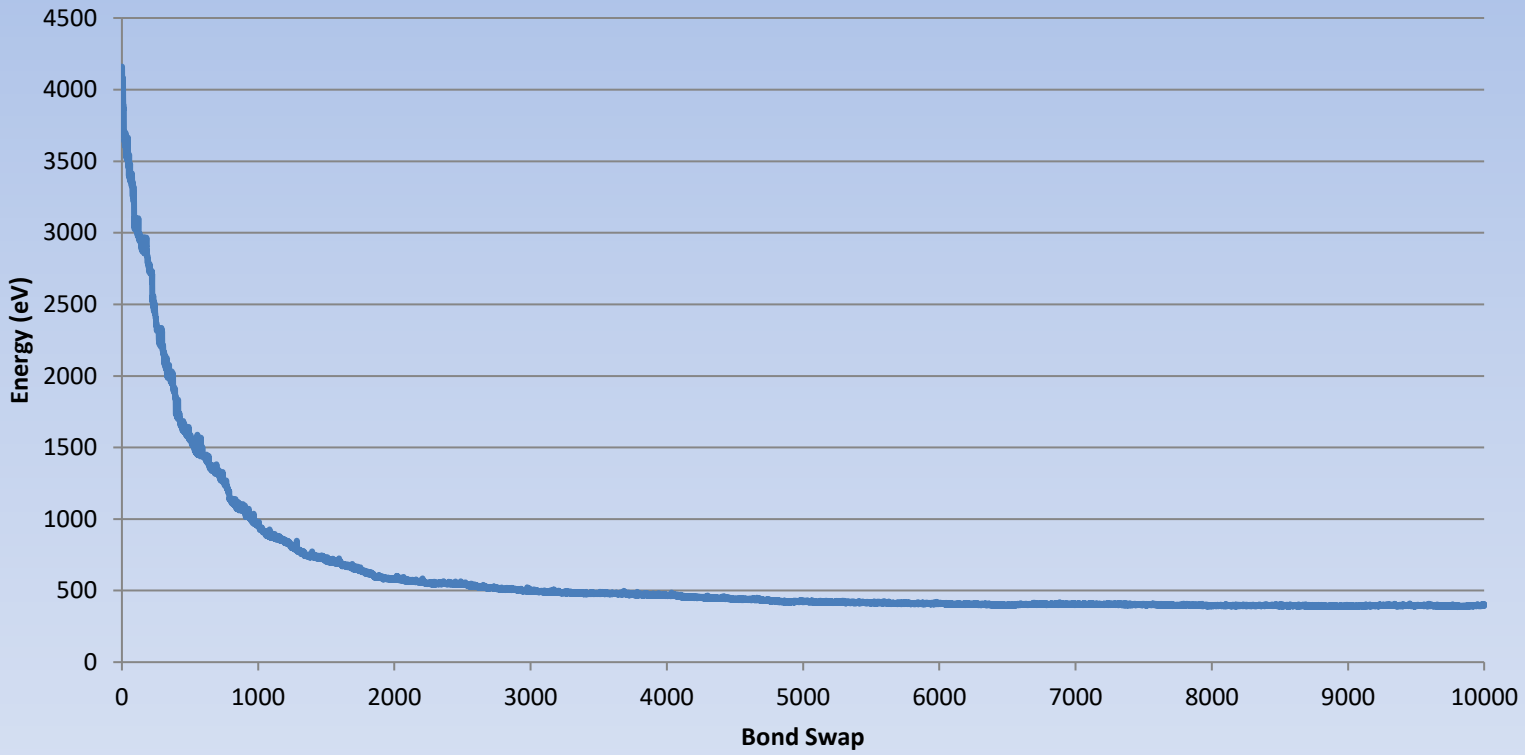
$$PE_{angular} = \sum_{i\in\alpha}\sum_{j\in\beta_i}\sum_{k\in\beta_i, k\neq j}\frac{1}{2}k_\theta\left(\cos\theta_{ijk} - \cos\theta_0\right)^2$$

$$PE_{repulsive} = \sum_{i\in\alpha}\sum_{m\notin\beta_i, \|\vec{r}_{im}\|<d_0}\sigma(d_0 - \|\vec{r}_{im}\|)^3$$

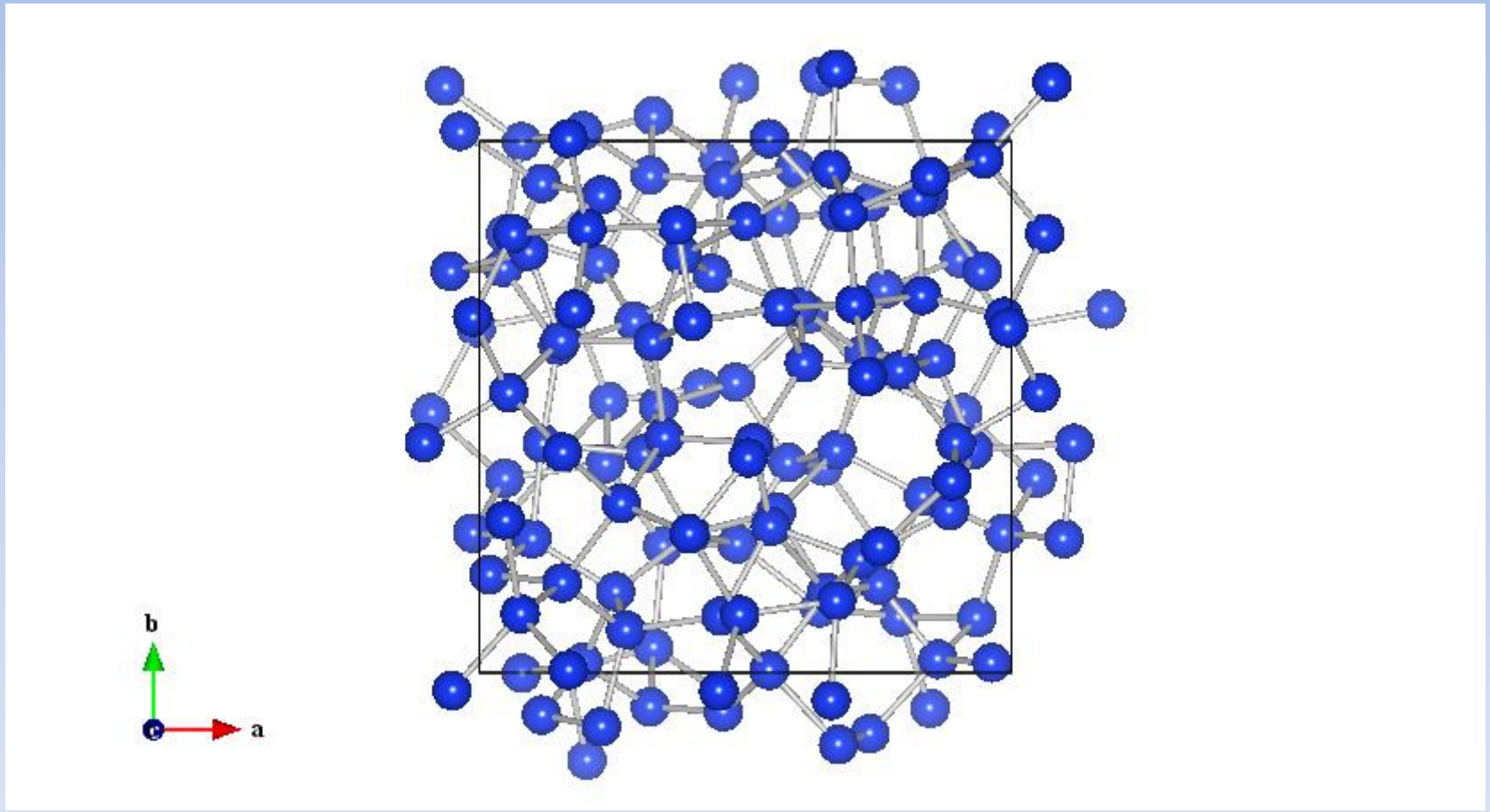
Simulation

- Bond swap
- Structure is relaxed using the Keating potential
- Metropolis Acceptance Probability (MAP)
  - $P = \exp[-\Delta E/\mathbf{kT}]$ if $dE > 0$, $P = 1$ if $dE < 0$

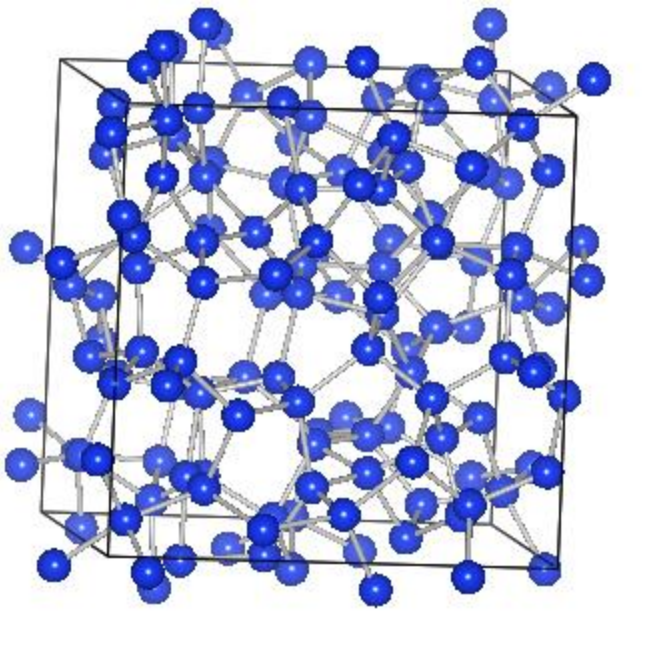
Energy vs. Number of Bond Swaps for One Cooling Run of the 216-Atom Crystal

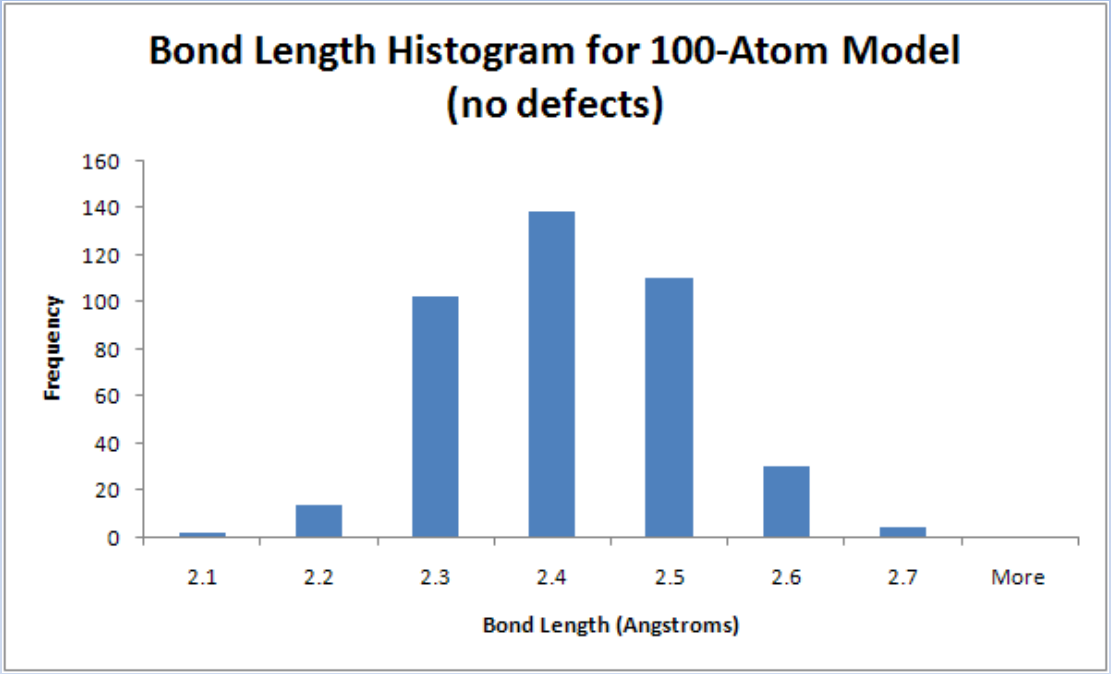


100 Si Atoms (kT=0.25)



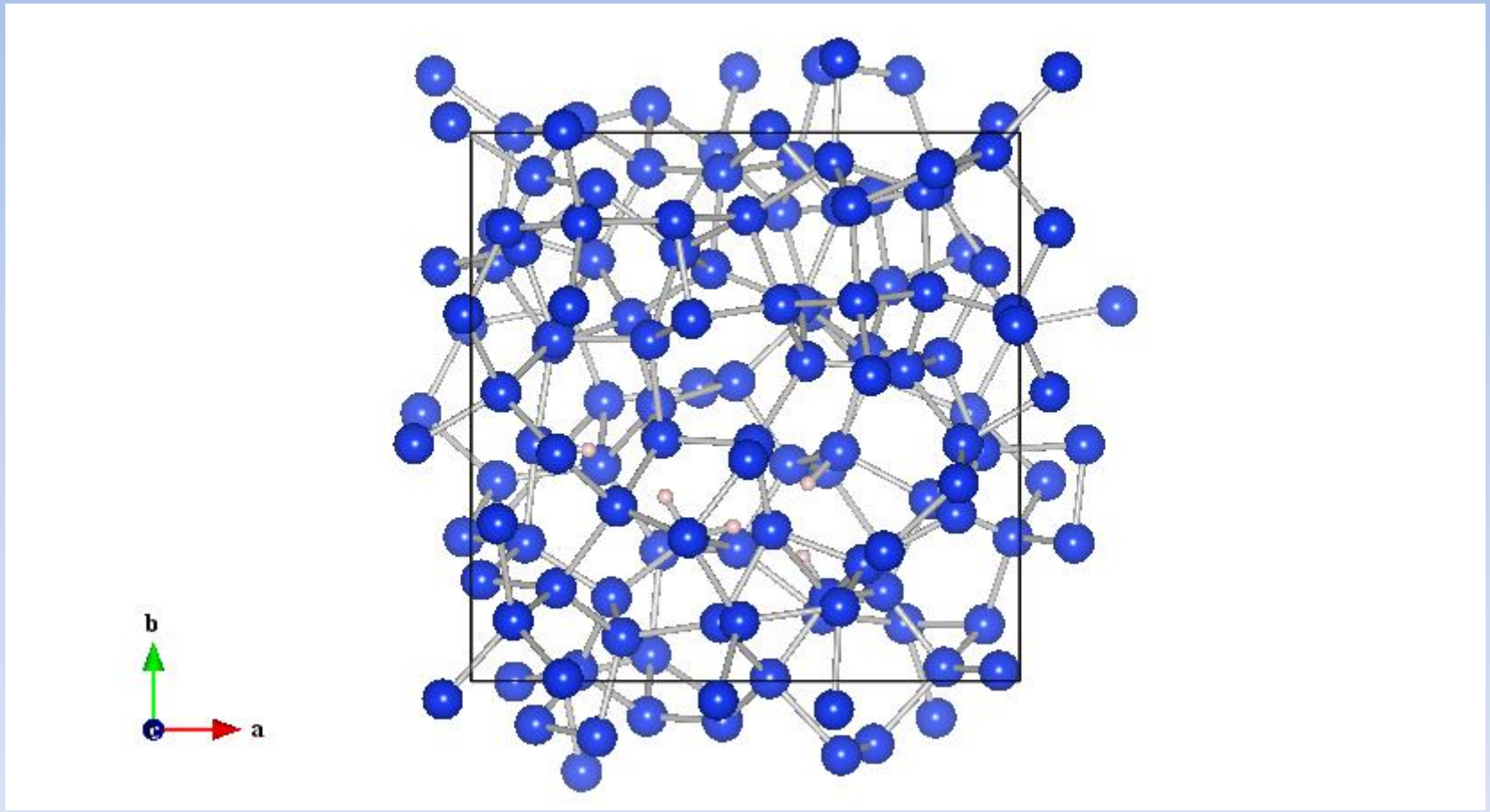
Final Model





*Generate models to study defects and H in amorphous Si

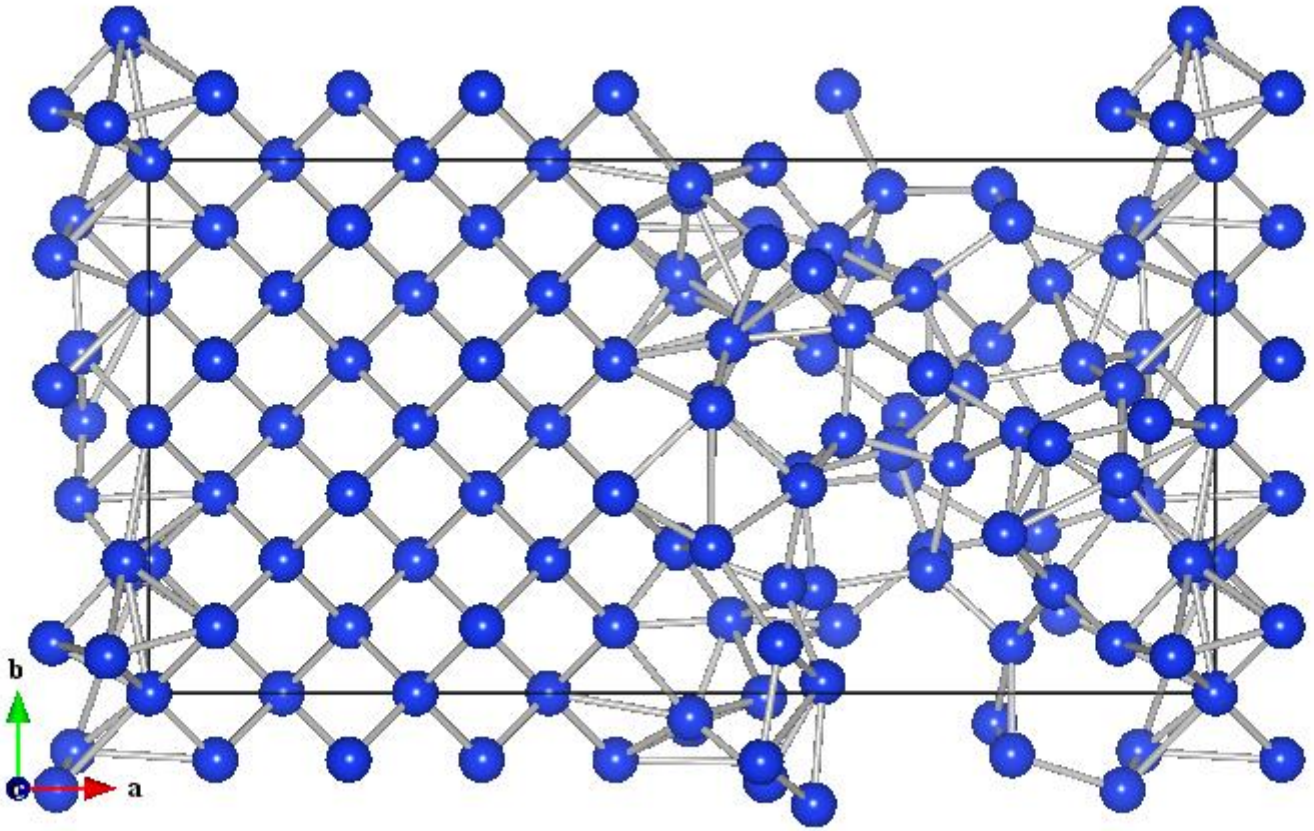
100 Si Atoms with Added H Atoms (kT=0.25)



Test Amorphous Si Model Data

#	N(Si)	E[BAM]	ΔE (VASP)	% ΔE
1	100	61	6.1	10.0
2	100	69	6.7	9.7
3	100	76	1.8	2.4
4	100	48	7.4	15.4
5	200	173 (87)	12.3	7.1
6	200	149 (75)	13.7	9.2
7	200	150 (75)	14.6	9.7

Crystalline Si / Amorphous Si Interface



Next Steps for Amorphous Si

- Analyze the electronic properties to ensure accuracy
- Calculate hyperfine parameters