

Optimization of Empirical Potential Parameters for Molecular Dynamic Simulation of Perturbed Si Crystal Configurations

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RESEARCH QUESTION:

IS THERE ONE SET OF EDIP POTENTIAL VALUES THAT WOULD GIVE “CORRECT” FORCES AND ENERGY VALUES FOR ALL DIFFERENT SI CRYSTAL CONFIGURATIONS CALCULATED BY MOLECULAR DYNAMICS ?



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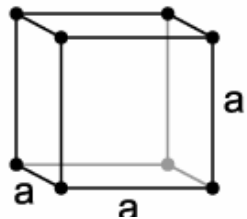


- EDIP FUNCTIONAL FORM:

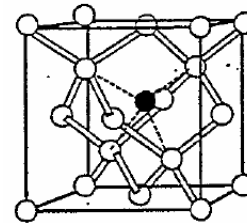
$$E = \sum E_i \quad i = 1 \dots N \text{ atoms,} \quad \text{Total energy of a configuration } \{ \vec{R}_{ij} \}$$

$$E_i = \sum_{j \neq i} V_2(R_{ij}, Z_i) + \sum_{j \neq i} \sum_{k \neq i, k > j} V_3(\vec{R}_{ij}, \vec{R}_{ik}, Z_i)$$

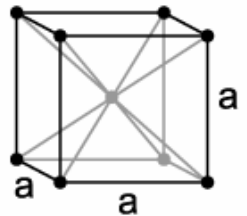
- BOTH TYPES OF ABOVE INTERACTIONS DEPEND ON THE LOCAL ENVIRONMENT OF THE ATOM WHICH IS DETERMINED BY ITS NEIGHBORS.



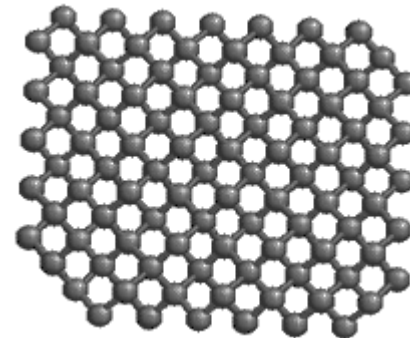
Simple Cubic



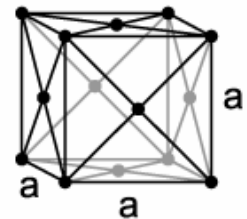
Perturbed FCC



Body-Centered Cubic



Diamond
Crystal
Lattice

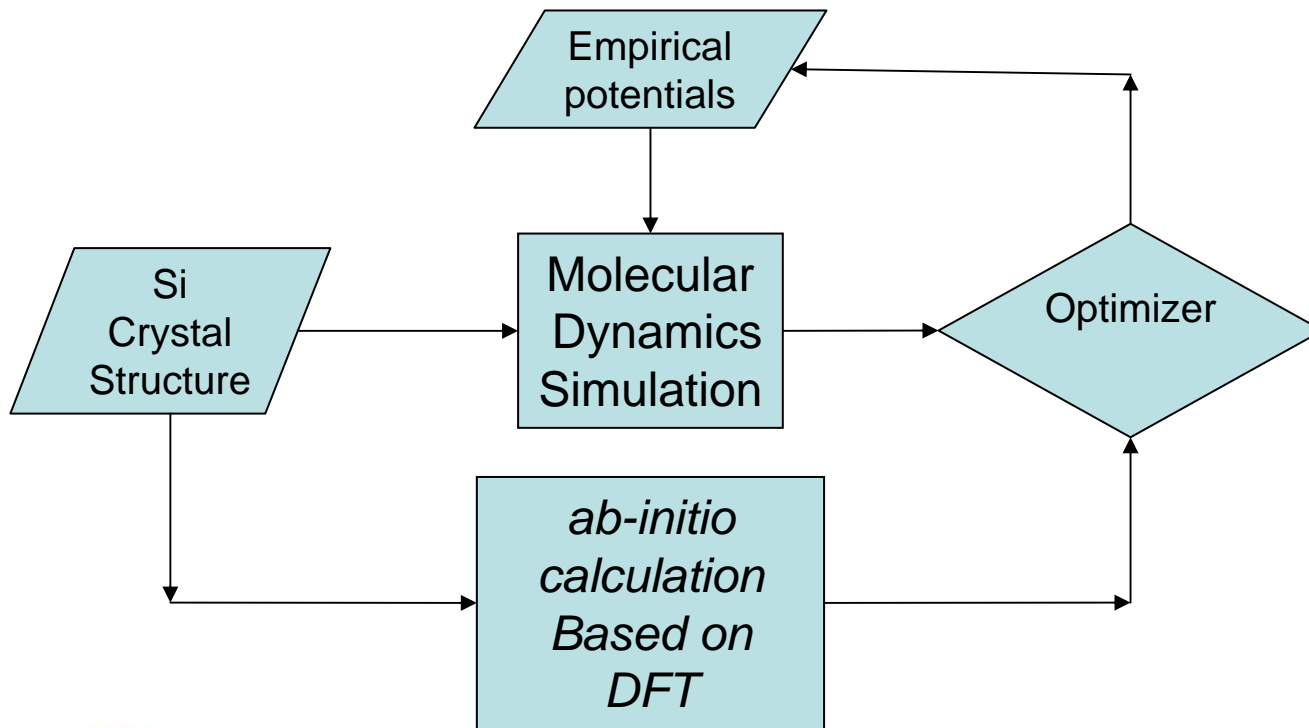


Face-Centered Cubic



PROBLEM ARRANGEMENT:

- PERTURBED SI DIAMOND CONFIGURATIONS WERE USED FOR TRAINING SET DATA.
- CONJUGATE GRADIENT ALGORITHM WAS USED AS OPTIMIZING TECHNIQUE.
- 15 EDIP PARAMETERS → 15 DEGREES OF FREEDOM!!!



RECENT RESULTS:

- SHOWED EXISTENCE OF AT LEAST ONE CONVERGENCE POINT FOR THE OPTIMIZER THAT IS REPRODUCIBLE.
- PRELIMINARY COMPARISON SHOWED THAT NEW OPTIMIZED EDIP PARAMETERS HAVE BETTER MD PERFORMANCE OUTSIDE THE TRAINING SET FOR PERTURBED BCC STRUCTURE.

FUTURE STEPS:

- LARGER TRAINING SET INFORMATION SHOULD BE INCORPORATED.
- PERFORMANCE COMPARISON WITH OTHER OPTIMIZING TECHNIQUES E.G. GENETIC ALGORITHMS, LEVENBERG-MARQUARDT
- MORE DETAILED COMPARISON OF PERFORMANCE OUTSIDE TRAINING SET SHOULD BE CONDUCTED.

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THANK YOU!



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