Genetic Algorithms for Surface Reconstruction

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I. 1997: Fu et al. [2]

- Si(001) surface - tight binding scheme
- Only the *top* layer undergoes GA steps
- periodic in x and y
- Map co-ordinates onto *binary* strings for crossover and mutation
- relax into local minimum through molecular dynamics quenching (600 time-steps = 0.6 ps)
- minimum found after 21 generations, and remained so for 65 (length of run)

II. 2002: Miyazaki and Inoue [3]

- looking at deposited structure of atoms
- Lennard-Jones
- $2^{10} \times 2^{10} \times 2^{10}$ mesh
- 30 bit strings
- used seeding technique to determine structures
- found LJ_{13} cluster
- low mutation rate = 0.0003, and recombination rate of 0.2
- substrate 10 layers with FCC(001) surface
- no periodic boundary conditions

III. 2004: Chuang et al. [1]

- Si(105) - empirical potential
- real space representation and crossover
- periodic in x and y, no periodicity in z
- only atoms in top 5 Å undergo genetic operations
- crossover with plane perpendicular to surface
- whole of structure (15-20 Å deep) is relaxed
- variable atom number
- atom number need not be held constant
- required less than 200 mating operations to give lowest structure
- future work: other high index Si and Ge surfaces

IV. OUR METHOD

- real space representation
- periodic in all directions
- crossover is periodic with cell
- allows for bulk and surface calculations
- variable atom number
- atom number not conserved

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[1] F. C. Chuang, C. V. Ciobanu, V. B. Shenoy, C. Z. Wang, and K. M. Ho. Finding the reconstructions of semiconductor surfaces via a genetic algorithm. *Surf. Sci.*, 573:L375–L381, 2004.

[2] R. T. Fu, K. Esfarjani, Y. Hashi, J. Wu, X. Sun, and Y. Kawazoe. Surface reconstruction of si (001) by genetic algorithm and simulated annealing method. *Sci. Rep. Res. Inst. Tohoku Univ. Ser. A-Phys. Chem. Metall.*, 44:77–81, 1997.

[3] K. Miyazaki and T. Inoue. Genetic algorithm simulation for deposited structure of atoms. *Surf. Sci.*, 501:93–101, 2002.