2013

The Construction of a Viscinal Ice Slab for Molecular Dynamics Simulations

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Introduction

Cirrus clouds are important for climate regulation due to their light scattering properties[1]. The light scattering properties of cirrus ice crystals are largely determined by their shape, the most common shapes being hexagonal columns and plates[2,3]. Molecular dynamics (MD) simulations are important in understanding the growth mechanisms of these shapes. Flat ice slabs produced by the Buch et al. code have previously been used in MD simulations (Figure 1) [4,5].

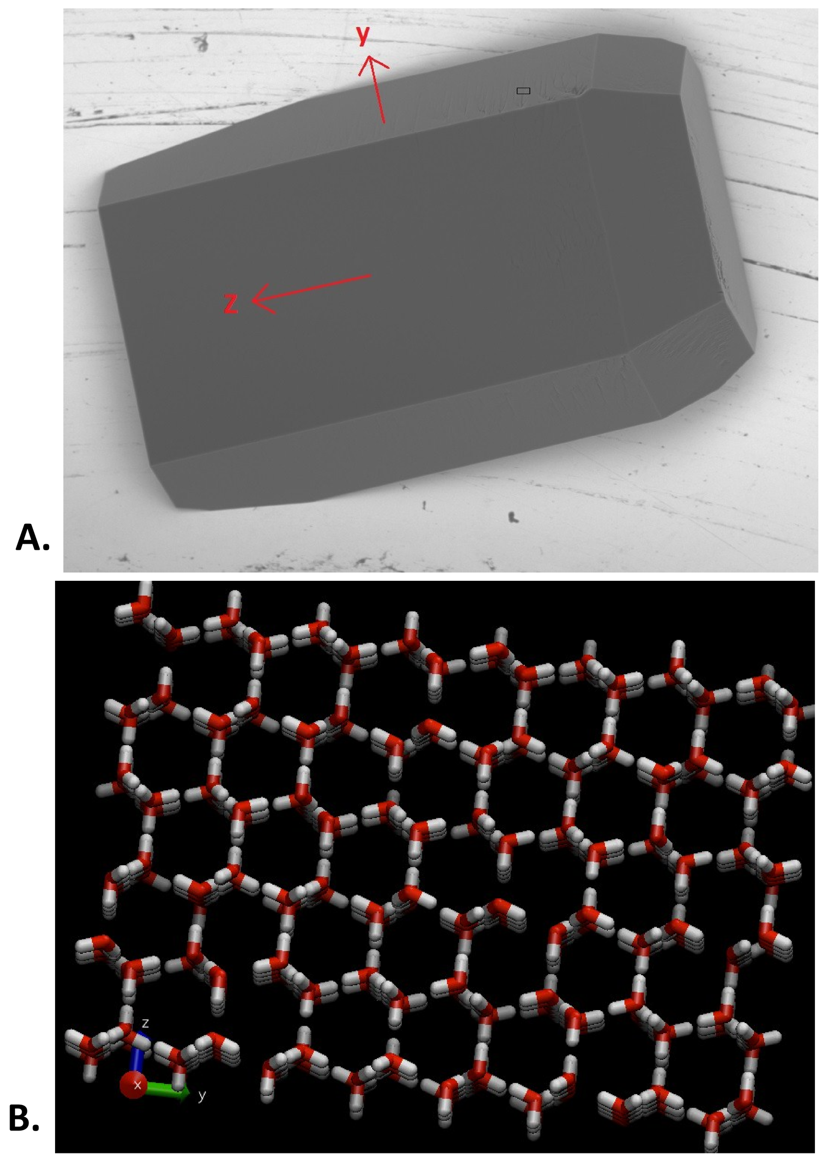

Figure 1. (A) A SEM image of a columnar ice crystal. (B) An MD representation of a flat ice slab produced in VMD

The Problem

Ice slabs used in MD must obey the Bernal-Fowler rules, also known as “Pauling’s ice rules,” while also satisfying the periodic boundary conditions (PBC). The ice rules refer to the fact that each individual oxygen within an ice lattice has four hydrogen bonds connected to it, two are hydrogen bond donating and two are hydrogen bond accepting(Figure 2).

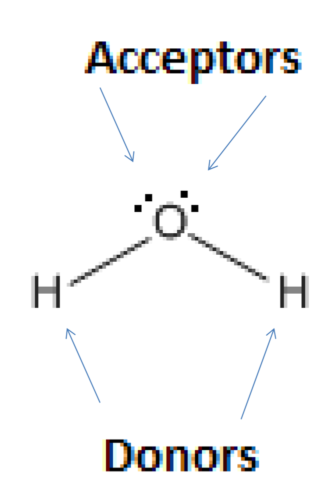

Figure 2. A water molecule obeying the Bernal-Fowler rules.

Constraints due to both the PBC and the ice rules have previously prevented a viscinal (roughened) slab from being used in MD (Figure 3).

Objective

Construct a viscinal slab using a protein data base file (.pdb) produced from the Buch et al. code that will satisfy the ice rules within the periodic boundary conditions.

Approach

- Identify nearest neighbors across a rotated (viscinal) slab.
- Propagate the defects (water molecules that do not obey the ice rules) through the ice crystal to the ice surface (Figure 3).

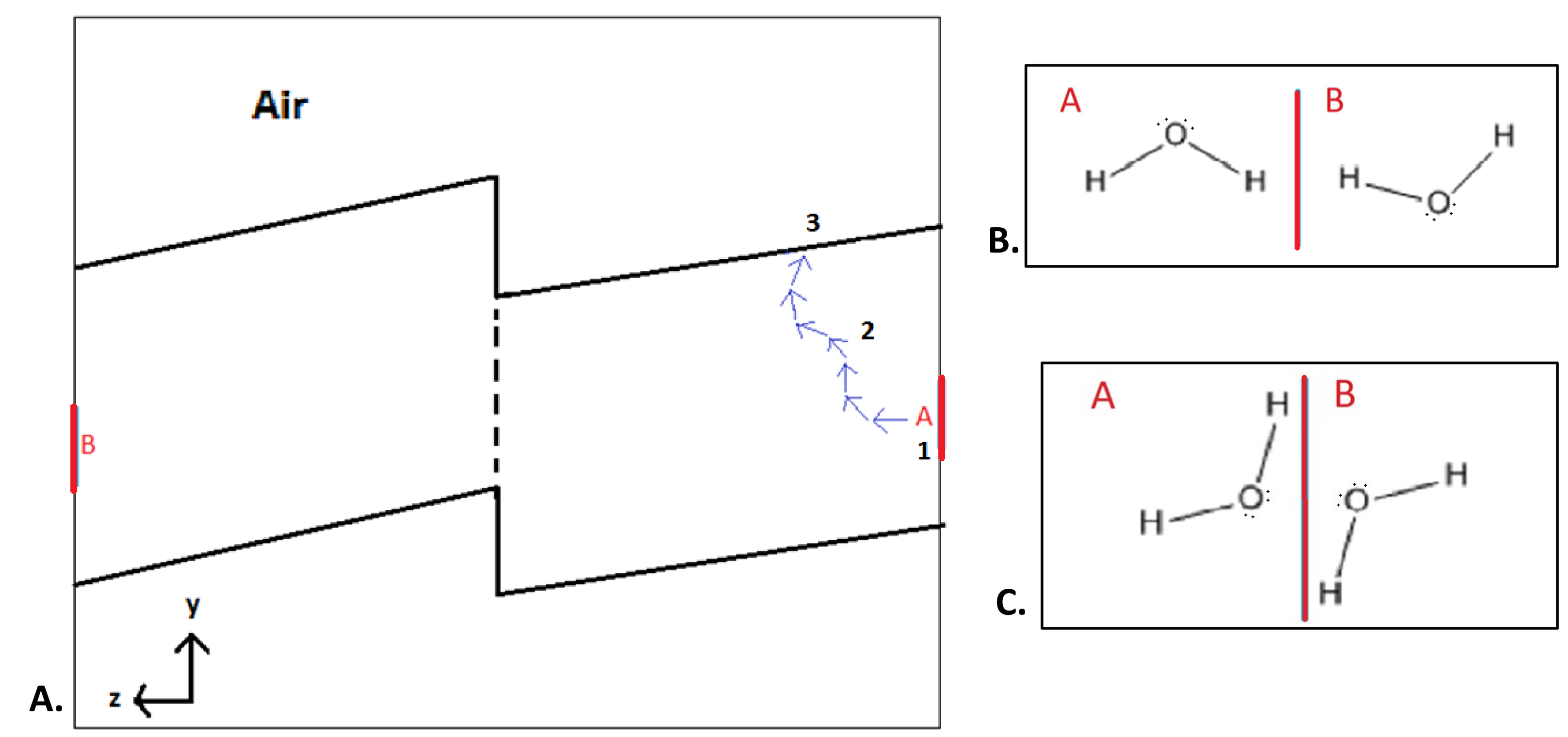

Figure 3. (Left) **(A).** A blown up cartoon image of the viscinal surface highlighted in Figure 1a. displaying the method of defect propagation used. (1) A defect between residue A and B is identified. (2) Propagate the defect through the ice crystal using a random-walk algorithm. (3) The defect reaches the surface and is fixed with a simple rotation along an axis to point the defect into the air. **(B).** A donor defect, Ddefect, across PBC. **(C).** An acceptor defect, Adefect, across the PBC.

Computational Strategy

- Using Enthought Canopy and Python, upload a .pdb file that yields a flat slab produced by the Buch et al. code.
- Apply a viscnal shift to the residues.
- Pull the coordinates of the Oxygen (O), Hydrogen 1 (H1), and Hydrogen 2 (H2) of each residue.
- Calculate the distances between all of the oxygen atoms in order to identify the four closest oxygen atoms, the “nearest neighbors,” (nni[i]) and identify where each residues’ Hydrogen atoms point (nnitol[i]).
- Identify all of the “defects” caused by the viscinal shift using nni[i] and nnitol[i].
- Fix the internal defects by propagating the defect through the ice crystal
- Fix the surface defects.
- Correct the actual coordinates using a rotation matrix.
- Output a new .pdb file.

Examples of nni[i], nnitol[i], and a Ddefect:

nni[3] = [4, 7, 15, -1]   nni[15] = [8, 3, 16, 20]
nnitol[3] = [1, 0, 2, 0]   nnitol[15] = [2, 1, 0, 0]

Ddefect:
3, 15

Results

We produced a viscinal slab that satisfies the ice rules within the periodic boundary conditions (Figure 4).

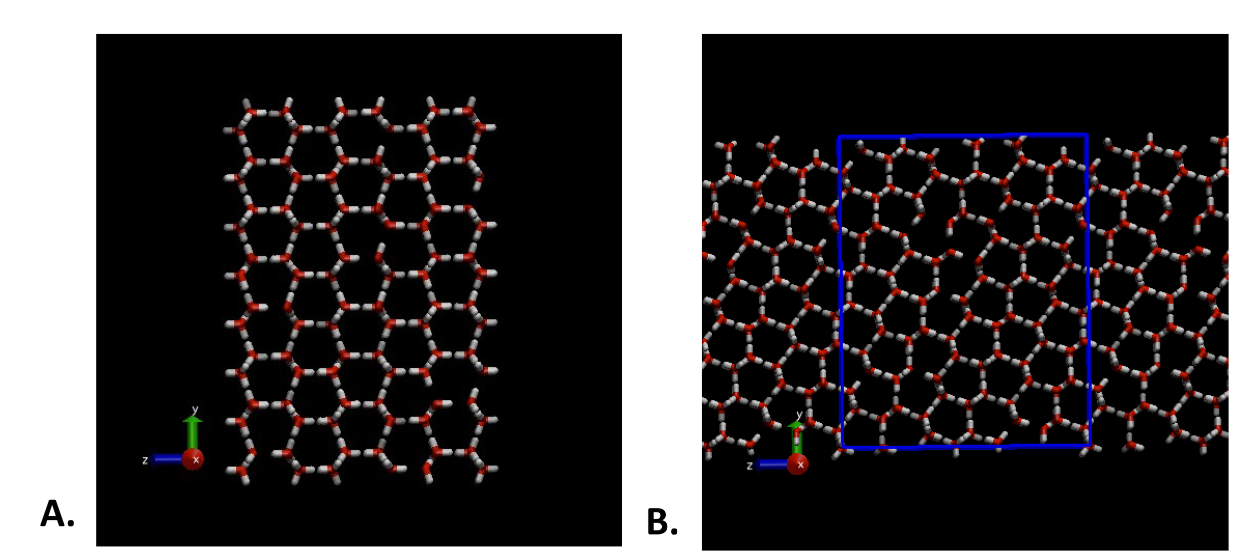

Figure 4. (Left) MD images of ice slabs produced in VMD. (A) a flat slab. (B) The new viscinal slab obeying the PBC.

References

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Future Directions

1. Improve the efficiency of the defect-removal algorithm
2. Carry out MD simulations of the dynamics of viscinal surfaces to measure key growth parameters, e.g., the step binding energy.