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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Scanning electron microscopy and molecular dynamics of surfaces of growing and ablating hexagonal ice crystals" *by* W. C. Pfalzgraff et al.

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We are grateful to the reviewer for suggesting that we take a closer look at geometrical aspects of this work. We now think there are two pyramidal prismatic facets, the predominant being the well-known 28-degree (101bar1) facet. The 14-degree has Miller-Bravais indices (202bar1), we believe. More details are given in our online comment to reviewer #1.

Regarding the stability (or transience) of the pyramidal prismatic facets, we rarely see a crystal that does not exhibit some development of this facet. We are currently trying to gather quantitative information about their incidence and extent, and whether those

properties depend on growth conditions (temperature, and ambient pressure to the extent that the VP-SEM allows).

As for the preference for prismatic attachment over basal attachment (to the copper substrate), our working hypothesis is that the crystal spacing of the copper substrate offers a better match to the prismatic facet.

Regarding the time dependence of relevant thermodynamic parameters, we have looked at the potential energy over time (Fig. 1 of this response). A feature around 5 ns – a reduction in potential energy – suggests (perhaps) a surface freezing process. We have not yet designed an approach that would allow us to pin down such structural changes, however. Perhaps a count of hydrogen bonds, or tracking the dipole correlation function? In our minds, a larger question is, what simulation scale is needed to reproduce the growth features seen in the SEM, and what approach might let us get to that scale?

Interactive comment on Atmos. Chem. Phys. Discuss., 9, 20739, 2009.

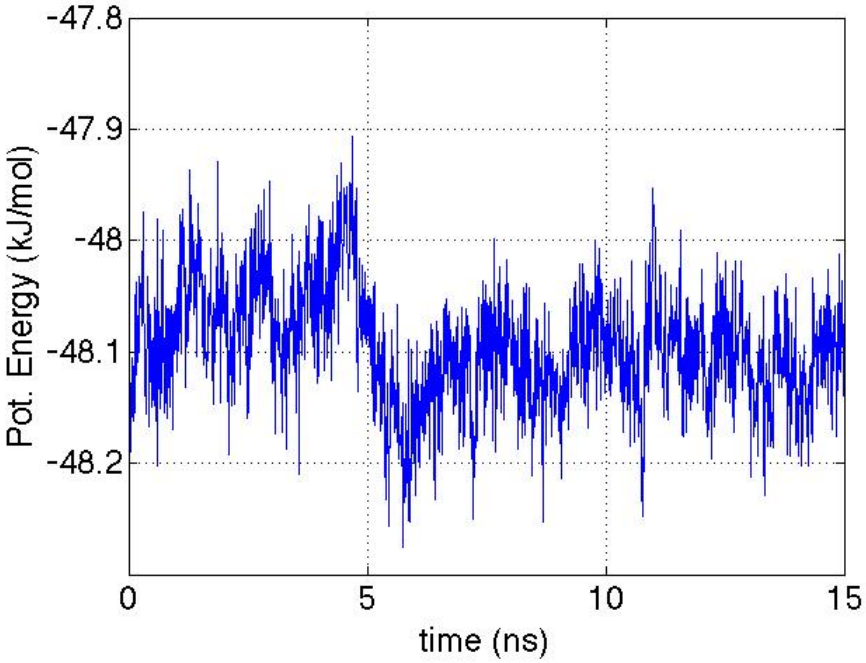

Fig. 1. Potential energy of the free-standing nanocolumn.