

Atmos. Chem. Phys. Discuss., referee comment RC2
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Comment on acp-2021-1054

Anonymous Referee #2

Referee comment on "Atomistic and coarse-grained simulations reveal increased ice nucleation activity on silver iodide surfaces in slit and wedge geometries" by Golnaz Roudsari et al., Atmos. Chem. Phys. Discuss.,
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This is an interesting paper that illustrates some of the complexities of heterogeneous ice nucleation on AgI by showing how the rate of nucleation in slits and wedges depends on the slit width and wedge angle. In a similar way to how AgI can enhance nucleation by providing a local matching template for ice growth, slits and wedges that provide a good match (e.g. by having a slit width that matches an integer number of ice bilayers) to the structure of the resulting ice crystal also enhance nucleation. I am happy to recommend publication once consideration has been given to the technical issues mentioned below.

1) Polar surfaces such as the AgI (0001) surface are well-known to be unstable in the absence of a polarity compensation mechanism. By keeping the ions in the AgI crystal fixed, this instability is avoided (albeit perhaps artificially), but it is important to consider how the electrostatic boundary conditions might affect the observed properties. Some discussion of these questions would be appreciated. The Sayer and Cox paper already referenced and J. Chem. Phys. **153**, 164709 (2020) are interesting in this regard.

2) By keeping the ions in the AgI crystal fixed rather than allowing them to exhibit thermal vibrations around their lattice positions provides a more perfect template for ice nucleation than would be expected if vibrations were allowed. Some discussion of how this potentially affects the results would be appreciated.