Supplementary Information

for

Surface effects on the crystallization kinetics of amorphous antimony

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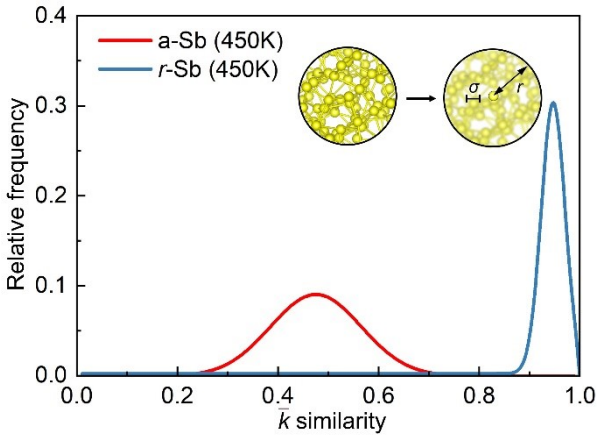

Figure S1. The distribution of calculated SOAP kernel similarity values for the amorphous bulk model and the *r*-Sb supercell model annealed at 450 K. The red and blue line represent the relative frequency of amorphous and crystal Sb environments at the elevated temperature, respectively, with a given kernel similarity to the reference structure (the idealized *r*-Sb supercell model at 0 K). The computed per-atom similarity $\bar{k}$ is given by averaging the similarities between the individual atom in the structural model and all the atoms in the reference structure.

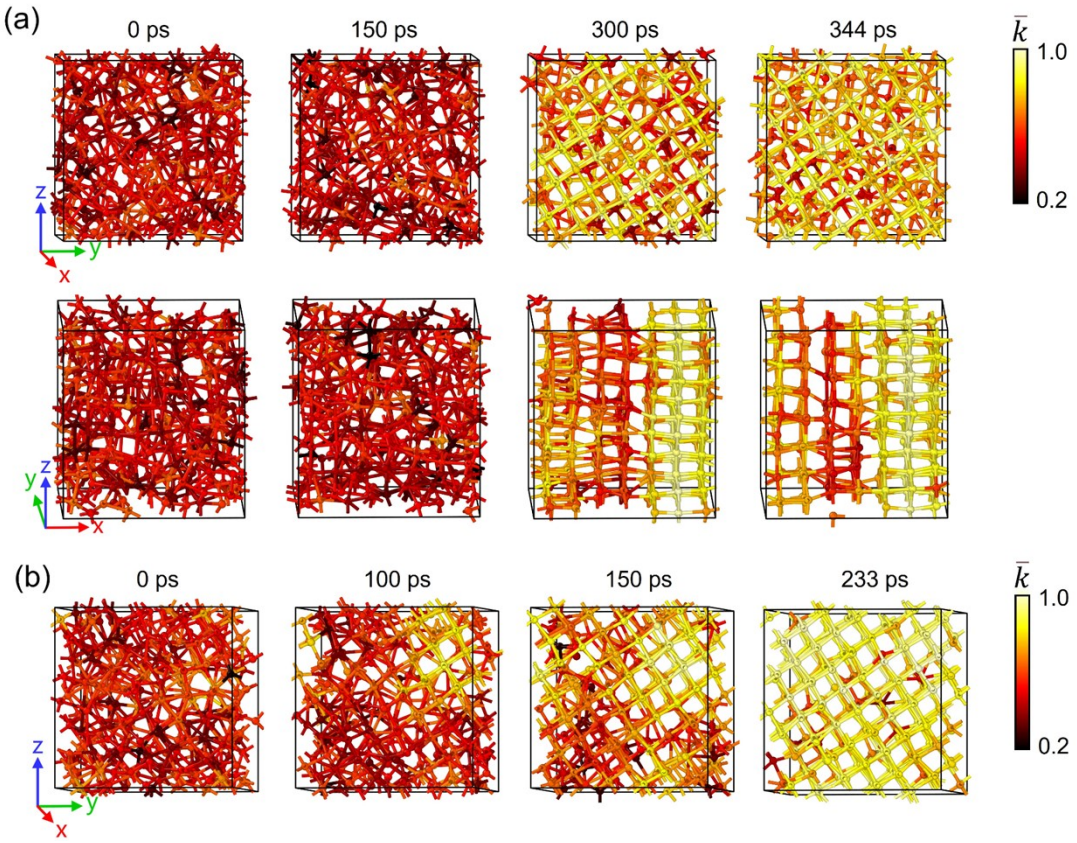

Figure S2. Structural snapshots of (a) bulk model **2** and (b) bulk model **3** taken at various time points during the crystallization simulation. Two different perspectives are shown for model **2**. Atoms are color-coded based on the calculated $\bar{k}$ similarity, which

quantifies the per-atom "crystallinity" with respect to the *r*-Sb supercell model.

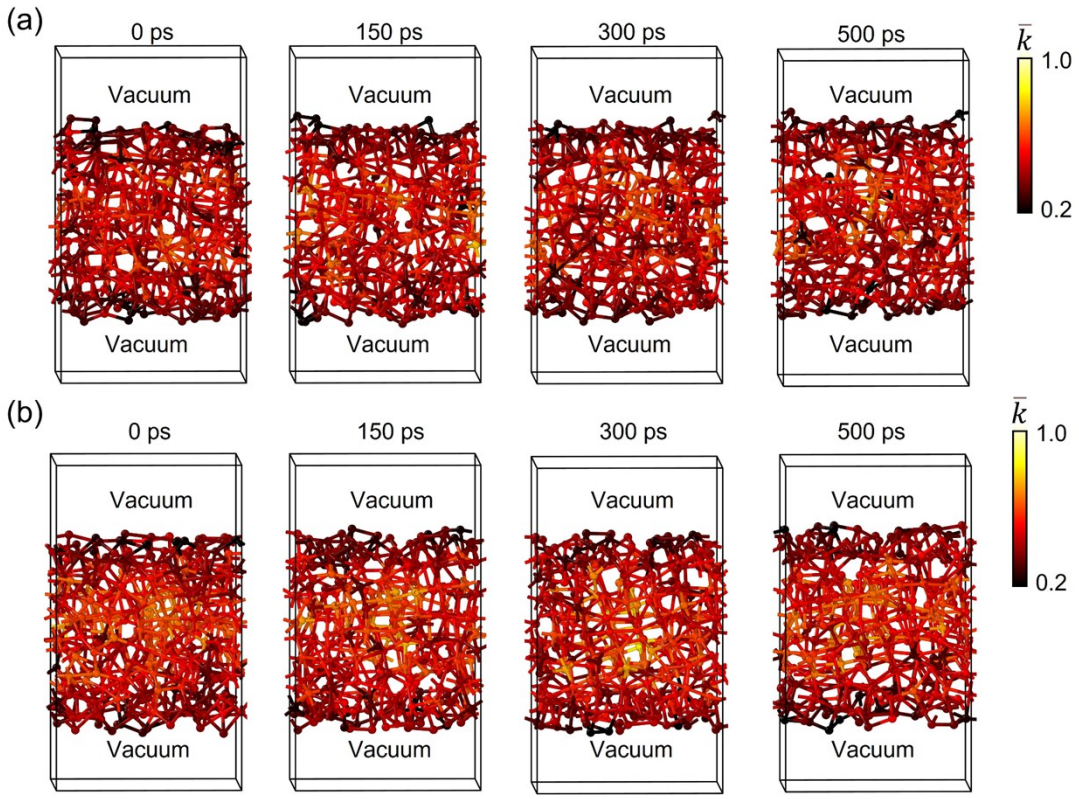

Figure S3. Structural snapshots of (a) surface model **2S** and (b) surface model **3S** taken at various time points during the crystallization simulation. Atoms are color-coded based on the calculated $\bar{k}$ similarity as in Figure S2.