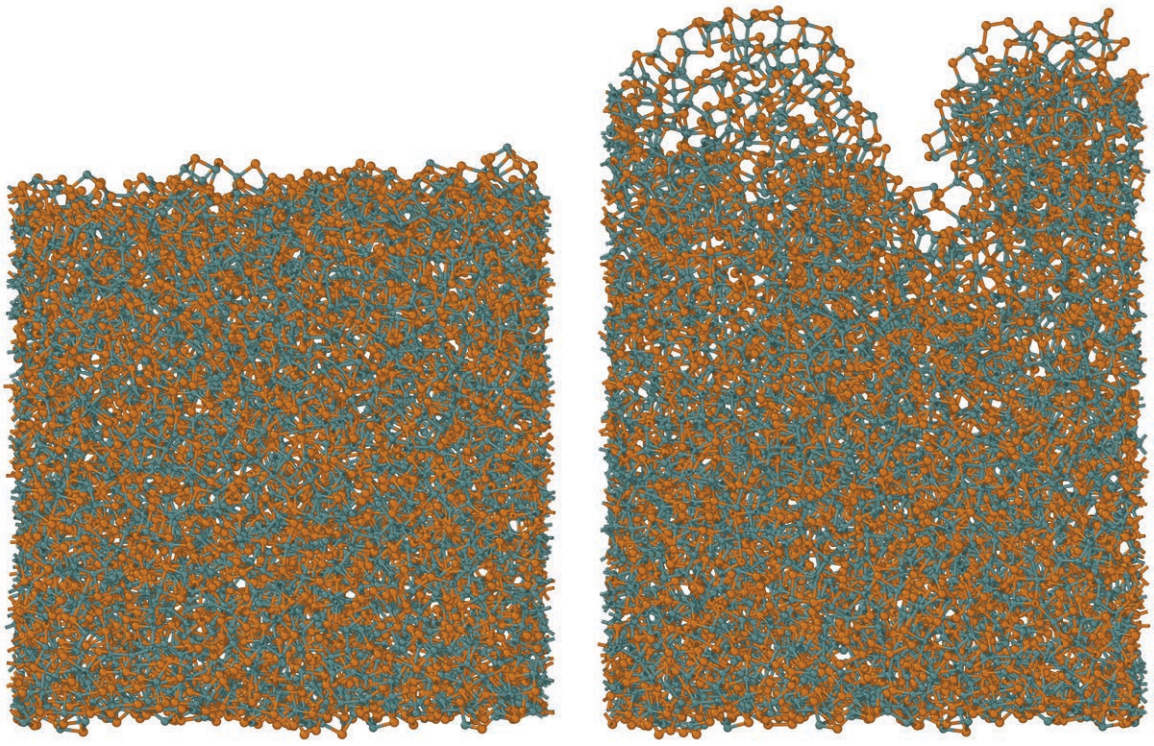
Structure and Crystallization Kinetics of as-deposited Films of the GeTe Phase Change Compound from Atomistic Simulations

SUPPORTING INFORMATION

*Simone Perego, Daniele Dragoni, Silvia Gabardi, and Marco Bernasconi**

Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Via R. Cozzi 55, I-20125 Milano, Italy

E-mail: marco.bernasconi@unimib.it



(a) (b)

Figure S1: A 7900-atom film obtained by depositing atoms with a) average kinetic of 5 eV (see Fig. 1c in the article) and b) average kinetic energy of 25 meV. The density of the film in panel b) is as low as 0.0252 atom/$\mathrm{\AA}^3$ due to the formation of a columnar morphology and voids.

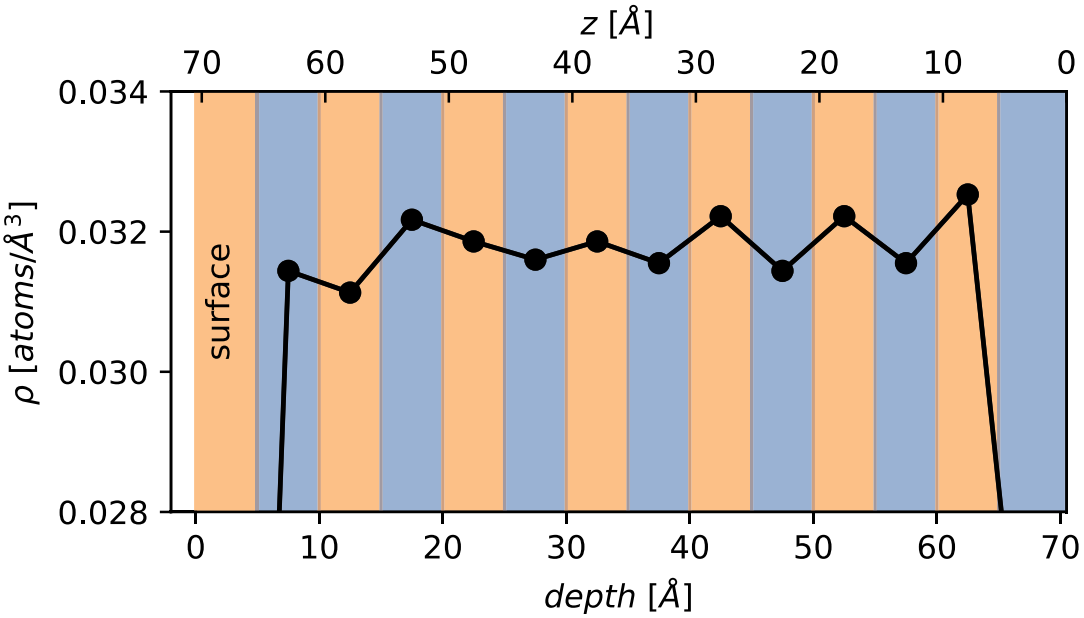


Figure S2: Local density as a function of the distance from the surface (depth) resolved for thin 5 Å slices in the AD-5 model.

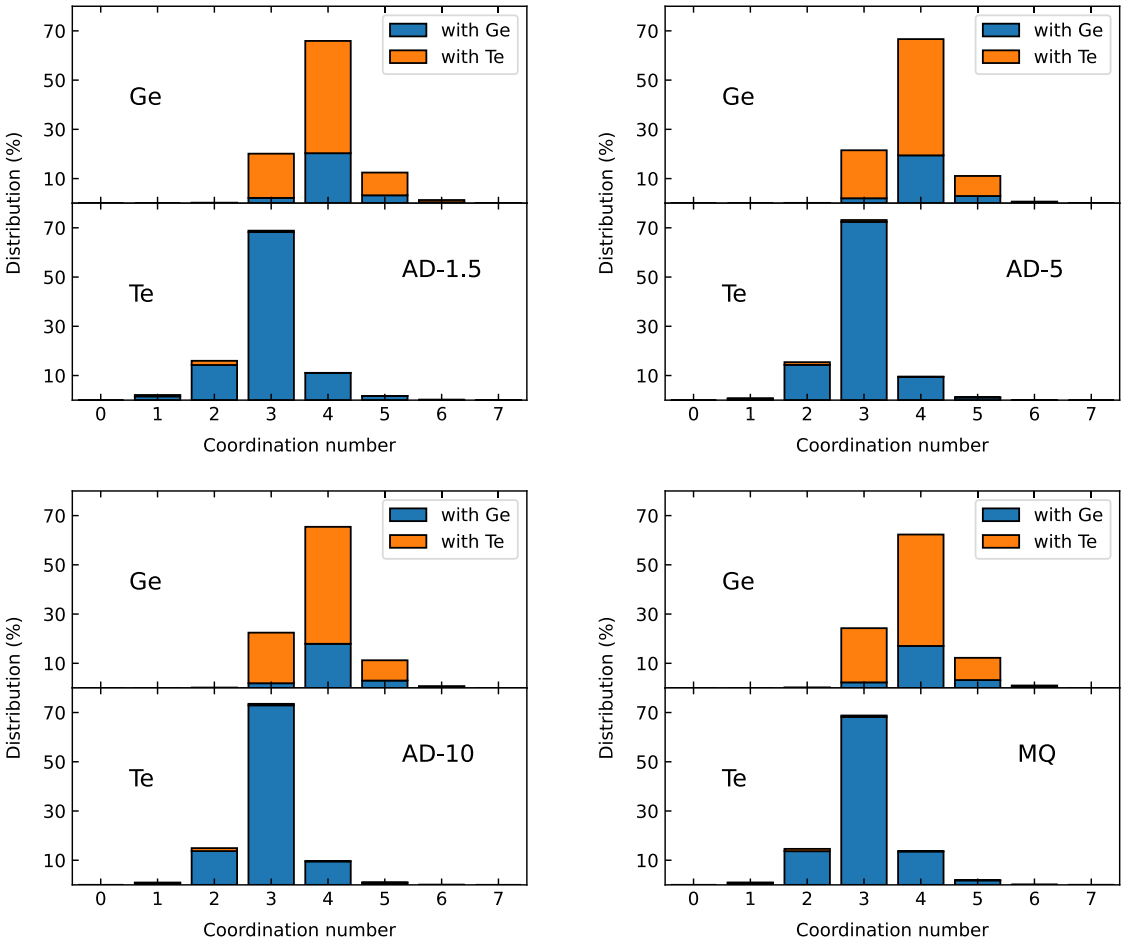


Figure S3: Distribution of the coordination numbers of deposited AD-1.5, AD-5, AD-10 models corresponding to different average kinetic energy of the deposited atoms compared with the data for the MQ model at the theoretical equilibrium density (see text in the article). The contributions from the different pairs of atoms are indicated by different colors.

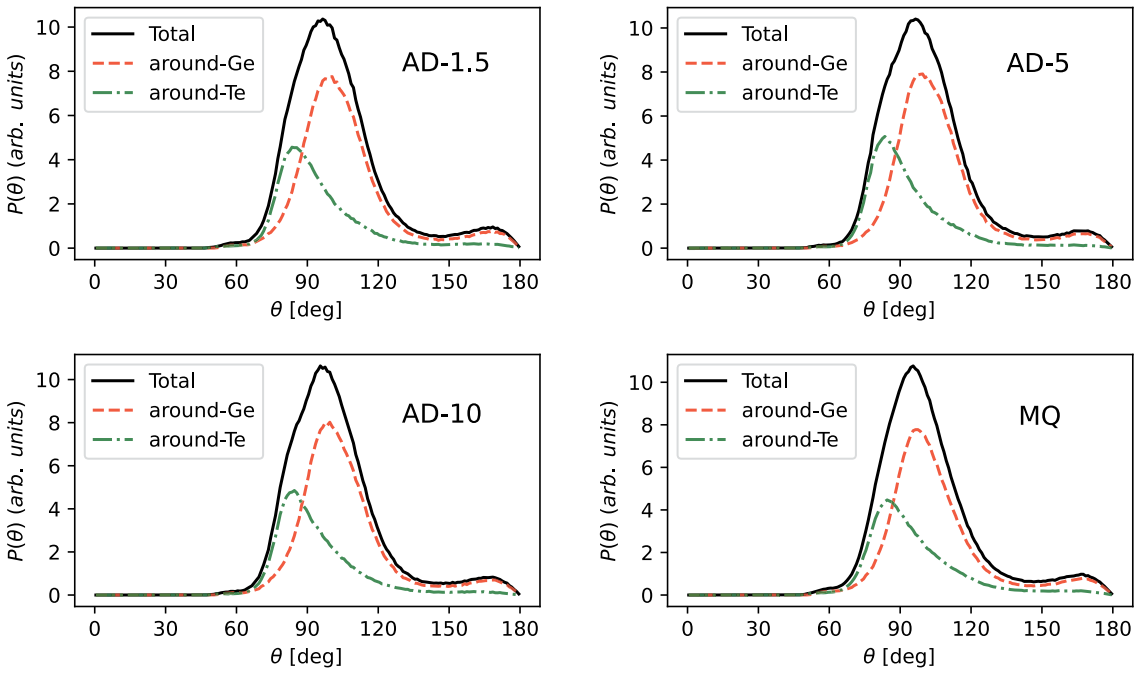


Figure S4: Bond angle distribution for the AD-1.5, AD-5, AD-10 models corresponding to different average kinetic energy of the deposited atoms compared with the data for the MQ model at the theoretical equilibrium density (see text in the article). The total distribution and the distributions resolved for the different types of the central atom are shown.

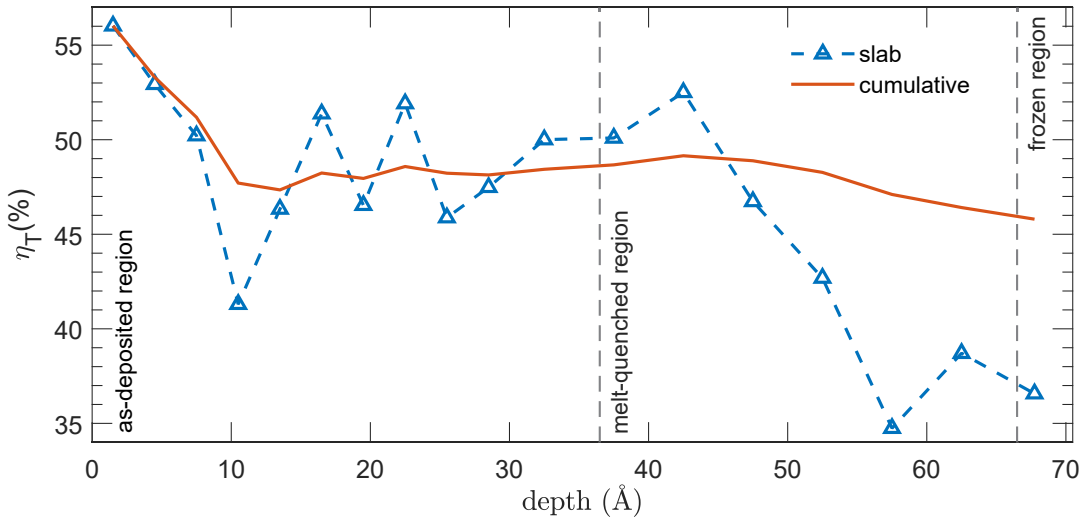


Figure S5: Percentage of Ge atoms in tetrahedral coordination with respect to the total number of Ge atoms as a function of the distance from the surface (depth) resolved for thin 3 Å slices in the AD-5 model. The percentage is calculated in each slice (blue triangles) and cumulatively starting from the surface (solid orange line).

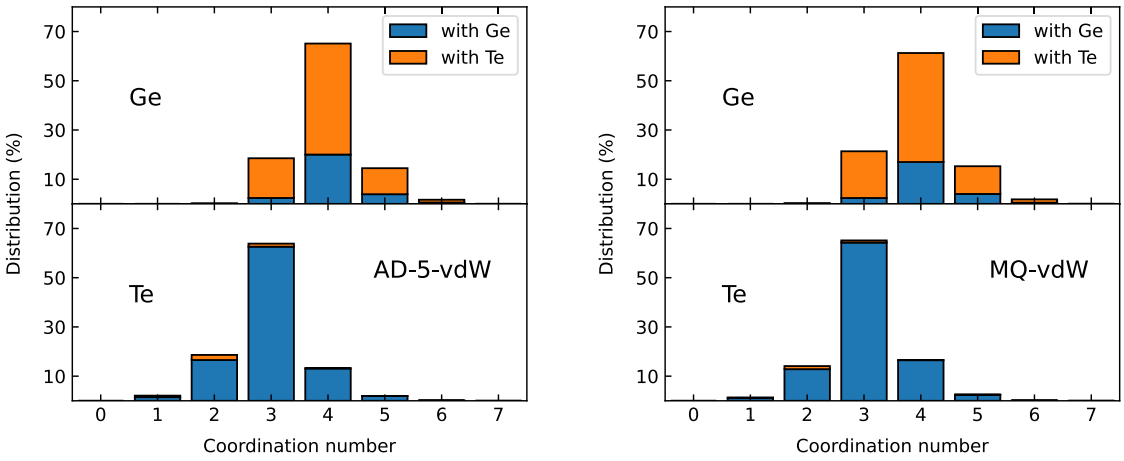


Figure S 6: Distribution of the coordination number of the deposited AD-5-vdW model generated with an average kinetic energy of the deposited atoms of 5 eV, compared with the data for the MQ-vdW model quenched from the melt at the same atomic density of the AD-5-vdW model (see text in the article). Both the AD-5-vdW and MQ-vdW models are generated by adding vdW interactions (see text in the article). The contributions from the different pairs of atoms are indicated by different colors.

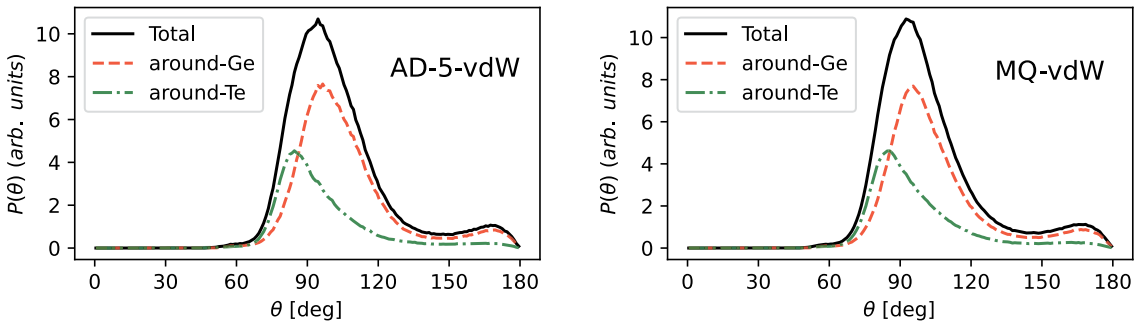


Figure S7: Bond angle distribution of the deposited AD-5-vdW model generated with an average kinetic energy of the deposited atoms of 5 eV, compared with the data for the MQ-vdW model quenched from the melt at the same atomic density of the AD-5-vdW model (see text in the article). Both the AD-5-vdW and MQ-vdW models are generated by adding vdW interactions (see text in the article). The total distribution and the distributions resolved for the different types of the central atom are shown.

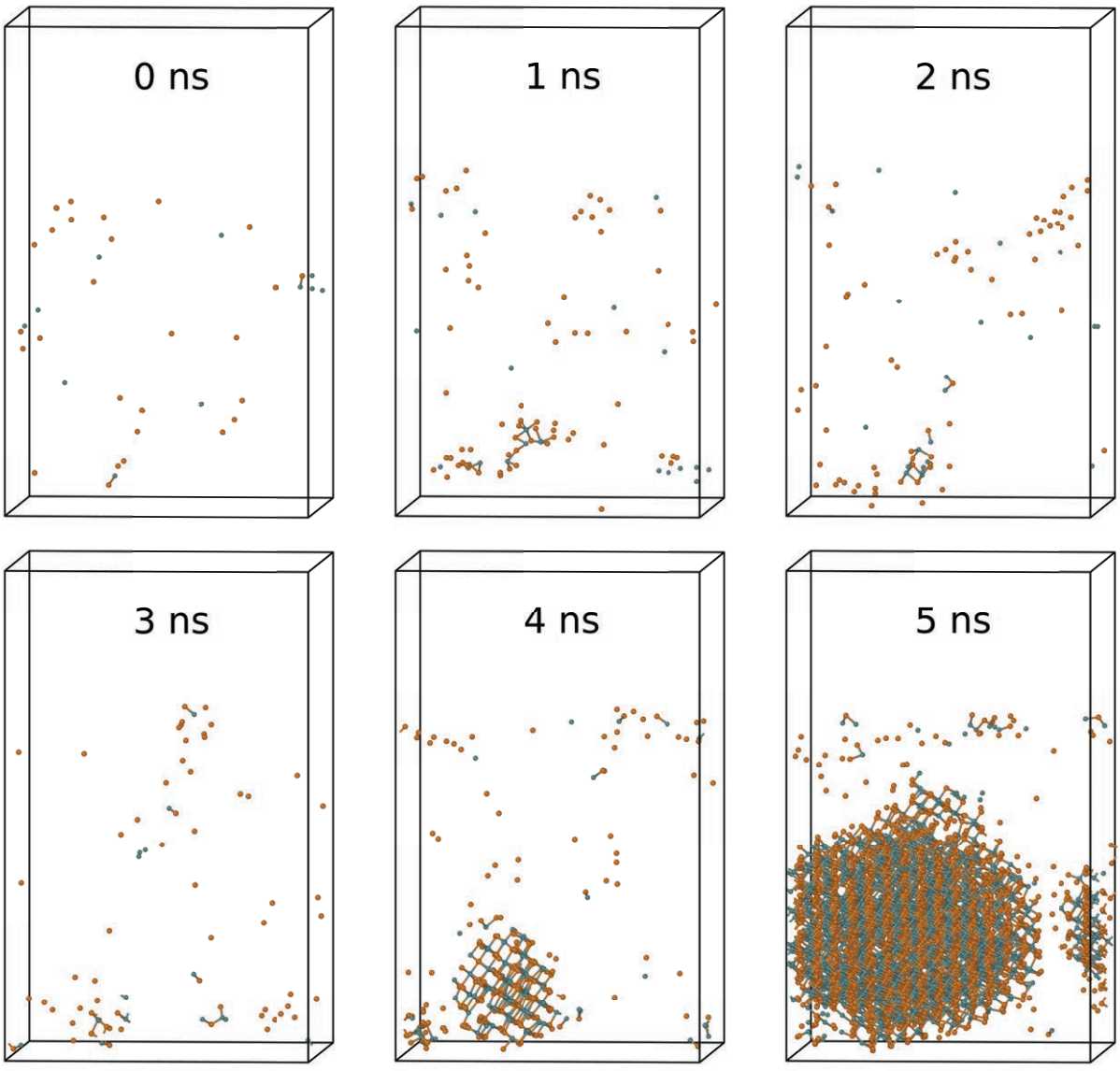


Figure S8: Snapshots of the crystalline atoms identified by the bond order parameter Q_6 (see Sec. II in the article) in the simulations of the AD-5 model at 600 K at different times. The bottom part is the substrate while the upper part is the free surface.

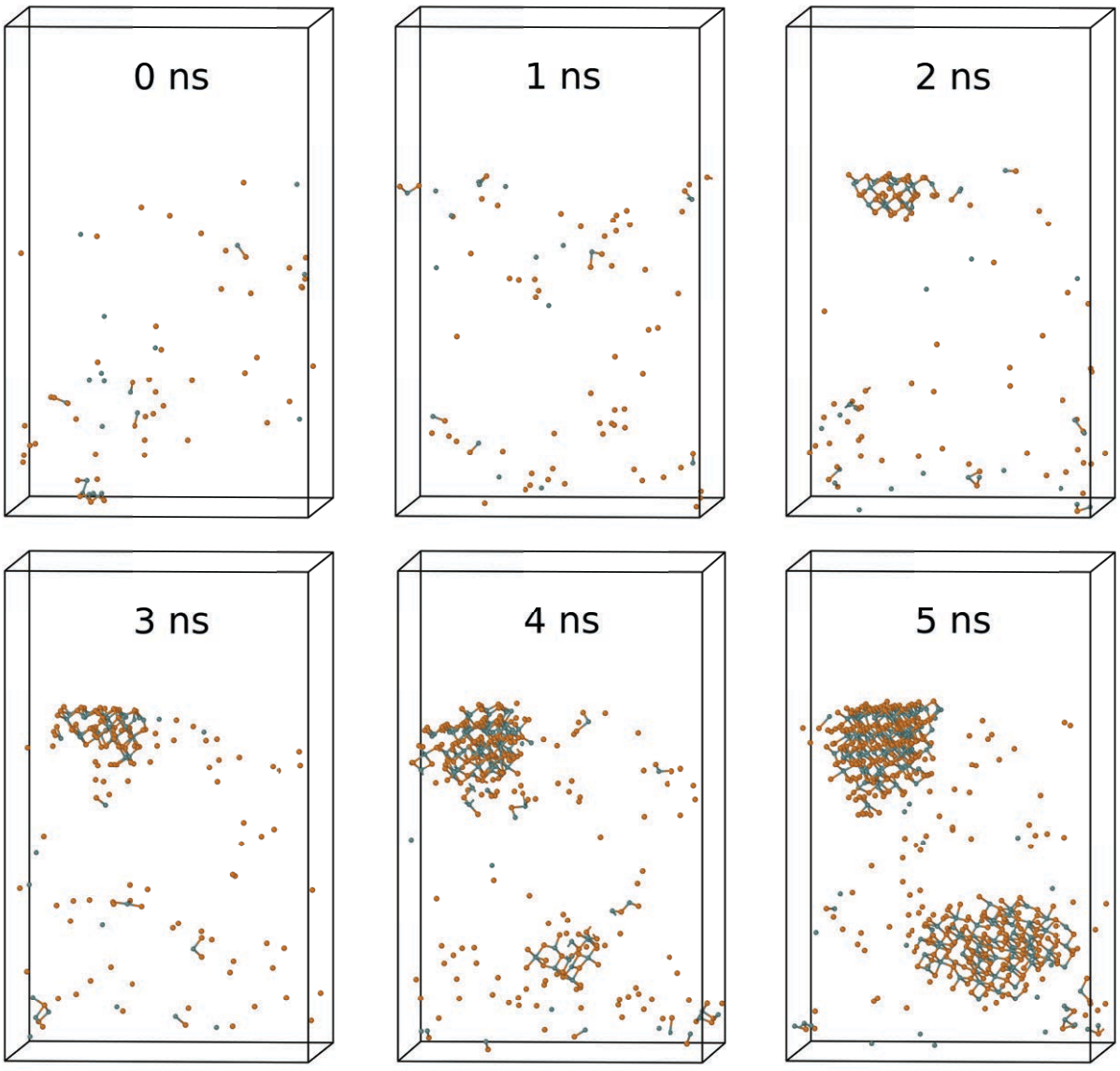


Figure S9: Snapshots of the crystalline atoms identified by the bond order parameter Q_6 (see Sec. II in the article) in the simulations of the AD-5 model at 550 K at different times. The bottom part is the substrate while the upper part is the free surface.

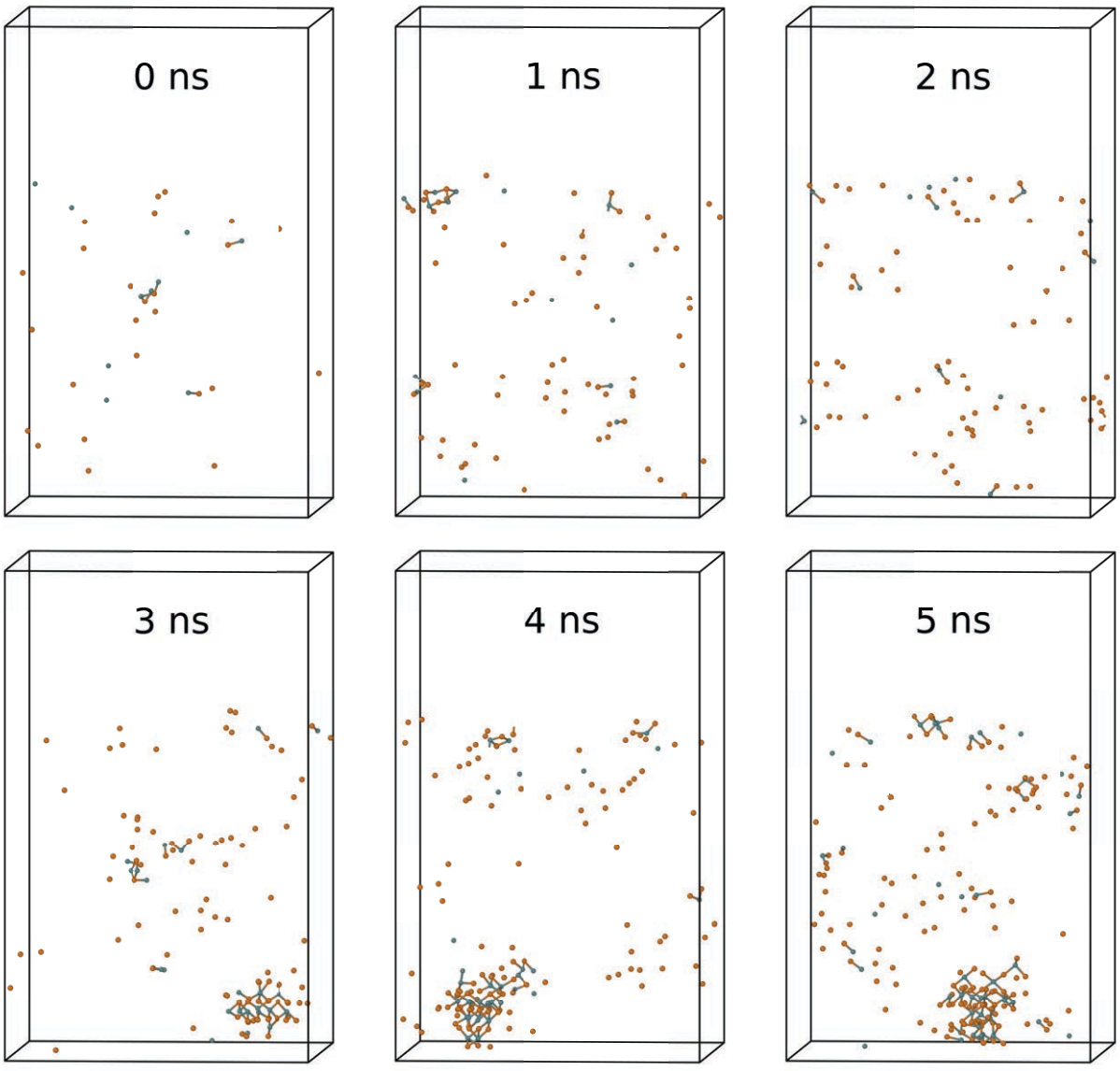


Figure S10: Snapshots of the crystalline atoms identified by the bond order parameter Q_6 (see Sec. II in the article) in the simulations of the AD-5 model at 500 K at different times. The bottom part is the substrate while the upper part is the free surface.

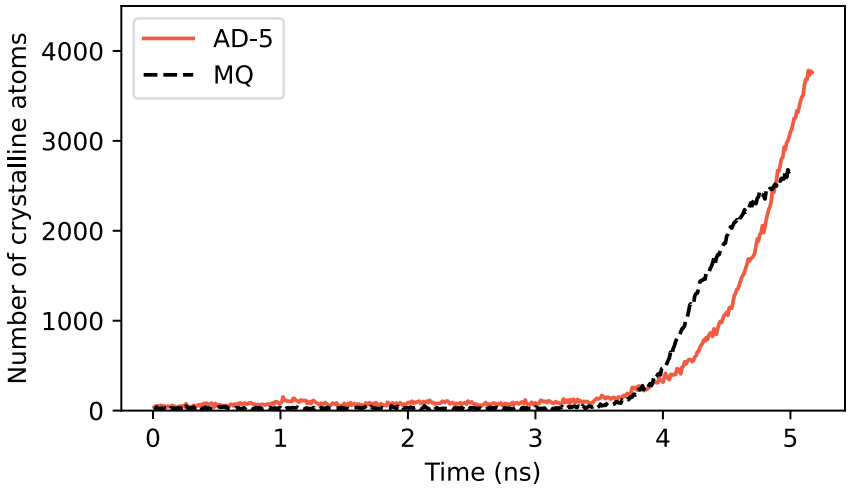


Figure S11: Evolution in time of the number of crystalline atoms during the crystallization at 600 K of the melt-quenched MQ (4000 atoms) and as-deposited AD-5 models (8000 atoms) with no vdW interactions.

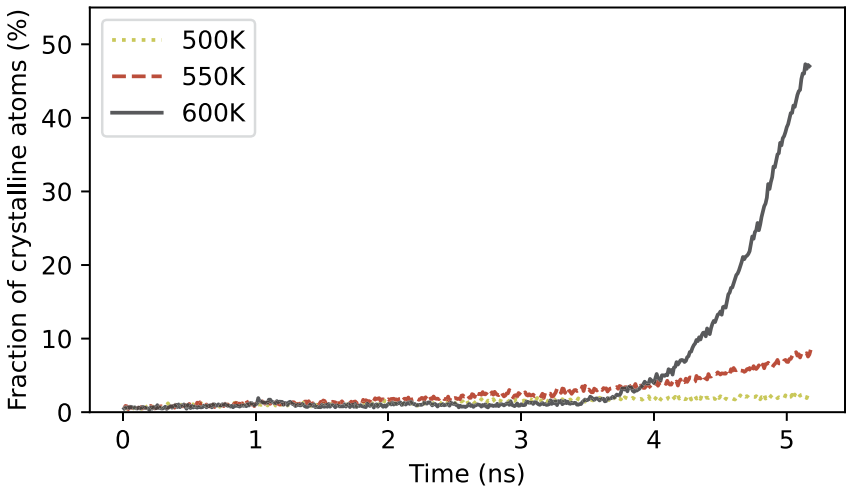


Figure S12: Evolution in time of the fraction of crystalline atoms during the crystallization of the as-deposited AD-5 model at different temperatures.

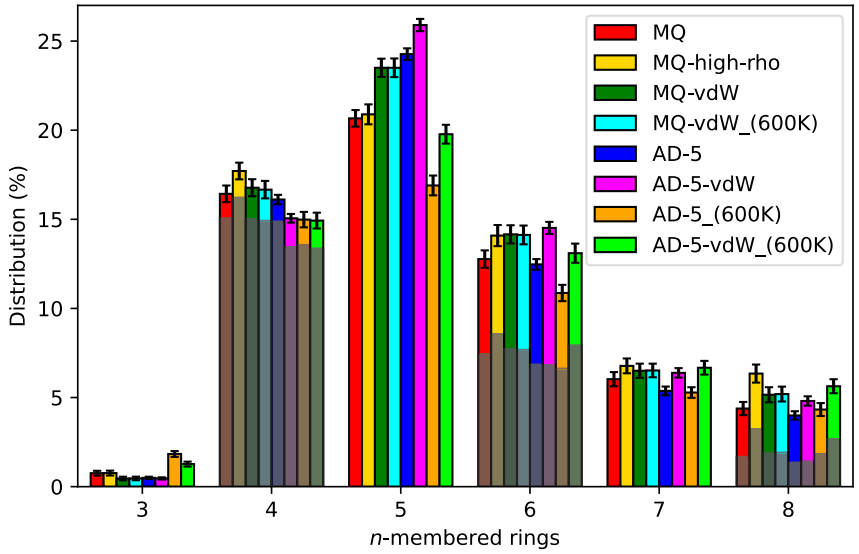


Figure S13: Distribution of ring lengths of the MQ models at different densities and of the AD-5 model. The data refer to simulation at 300 K or, where specified in the labeling, at 600 K before crystal nucleation takes place. Data for simulations including van der Waals interactions (vdW) are also reported (see text in the article). Darker region in each histogram with an even number of atoms refers to ABAB rings (A=Ge, B=Te). The distribution for AD models is computed for the whole model including the substrate.

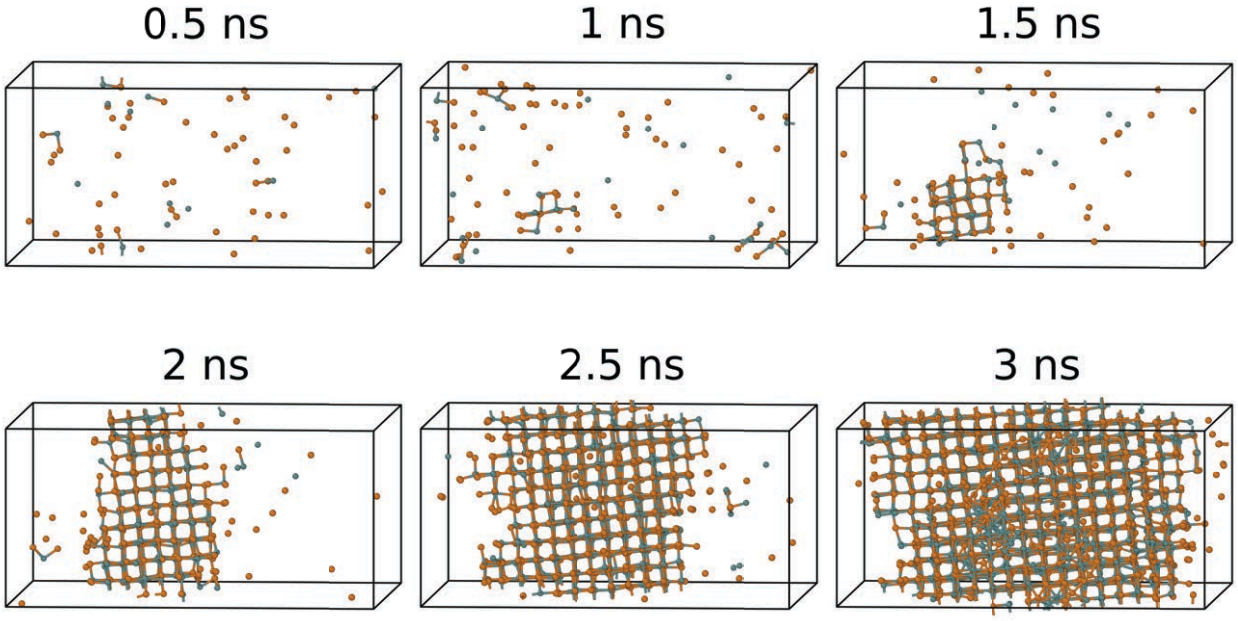


Figure S14: Snapshots of the crystalline atoms identified by the bond order parameter Q_6 (see Sec. II in the article) in the simulations of the MQ-vdW model at 600 K at different times.