Simulation Data used in the publication:
"Crystalline Morphology Formation in Phase-Field Simulations of Binary Mixtures"
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The root folder ("**512x512_dx1e-09/**") contains all the relevant data presented in the article, including simulation videos, post-processing data and final article figures.

Three types of subfolders can be distinguished within the root:

1) Folders containing simulation results (post-processing figures and videos) from the parameter space exploration study (Folders ending with "**...Var/**"),

2) Folders containing additional simulation cases used for further analysis of the different crystallization regimes ("**ExampleSpinoAssistedCryst/**", "**ExampleMpsiDDep/**", "**SingleComponentReference/**", "**SearchForRepellingCrystals/**", "**Eps1e-05_Kap1e-10_Mpsi100/**"),

3) Folders containing figure material used in the article (Folders: "**Article_Figures/**").

Furthermore, a supplementary "**Simulation_Database.csv**" file contains the list of all simulations produced for this work associated with their respective paths in the folder structure and their respective input parameter list.

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Folder type 1:

- The folders ending with "**...Var/**" contain the simulation results from the parameter sensitivity study (see Fig.5, Sec.4.2 in the article). The parameter which was varied is specified in the name of the folder, i.e.:

"Eps" and "Kap": the surface tension parameters "epsilon" (in sqrt(J/m)) and "kappa" (in J/m) which are involved in the processes controlled by the Allen-Cahn and Cahn-Hilliard equations, respectively. Note that the value intervening in the Allen-Cahn equation is actually Eps^2 and that "kappa" in the Cahn-Hilliard equation as it is written in the article corresponds to 2*Kap.

"Lfus" and "Wfus": the thermodynamic parameters of the latent heat of crystallization and the crystallization energy barrier (both in J/kg), respectively.

"Khill" and "Khisl": the amorphous-amorphous and amorphous-crystalline interaction parameters, respectively.

"Mpsi" and "D": the kinetic parameters "M0" (in 1/s) and "Lambda0", which control the dynamics of the Allen-Cahn and Cahn-Hilliard equation, respectively.

"N1_N2": the relative size of the species 1 and 2 on the Flory-Huggins lattice. In the SI of the article, only results for N1>=1 and N2=1 are presented since varying these parameters to values where N1=1 and N2>1 implies a change of the Flory-Huggins lattice element volume, which also has cross-effects with other energy contributions related to Khill and Khisl.

- Within the "**...Var/**" folders, intermediate subfolders specify the value of the parameters "Eps", "Kap" and "Mpsi" since different combinations were sometimes tried out to observe their impact on the sensitivity to paramter variations. Note that all results finally presented in the article are in folders "**Eps1e-05_Kap1e-10_Mpsi0p1/**", except of course when one of these three parameters was varied. In this case, the value of the variable is replaced with "Var" in the subfolder name, for instance "**Eps1e-05_KapVar_Mpsi0p1/**".

- Within the "**Eps..._Kap..._Mpsi.../**" folders, the results are again gathered in different subfolders following the value of the parameter for which the sensitivity of the crystallization kinetics is studied. For example, for the sensitivity of the crystallization kinetics to variations of "kappa", the folders "**Kap7e-11/**", "**Kap8e-11/**", "**Kap9e-11/**" "**Kap1e-10/**", etc... can be found under the "**KapVar/Eps1e-05_KapVar_Mpsi0p1/**" folder structure. (Note that the subfolders related to the study of "Lambda0" are here named after the scaled values of the self-diffusion coefficents of species in pure material systems rather than the value of "Lambda0" directly, e.g. "**D[1e-13_5e-10_1e-12_2e-09]/**" rather than "**D1/**". This is different in folders of type 2.)

- Within one of these latter subfolders, one finds the simulation data for each simulated blend ratio between phi0 = 0.2 and phi0 = 0.99. The name of a simulation (which is abbreviated with **<SimName>** below) consists of a list of the relevant simulation parameters and reads either
"**CrystInBlend_2D_PCBM-DCB_Mesh512_dx1e-09_T333K_Phi..._PowCryst1_Lfus..._Wfus..._Eps..._Kap..._D[..._..._..._...]_Mpsi..._Khill..._Khisl..._ACNoise1_CHNoise0**"
or
"**CrystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi..._PowCryst1_Lfus..._Wfus..._Eps..._Kap..._D[..._..._..._...]_Mpsi..._Khill..._Khisl...**"

- For each simulated blend ratio, the simulation data consist of one folder "**<SimName>/**" which contains the video of the simulated progress of crystallization along with post-processing data such as figures of the time-evolution of different quantities of interest.

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Folder type 2:

- The folder "**ExampleMpsiDDep**" contains additional simulations of crystallization in dilution-enhanced systems (which are potentially also diffusion-limited, depending on the value of "Lambda0"). The figures presented in the article base on the results contained in the "**Eps1e-05_Kap1e-10_MpsiO0p1/**" folder. There, additional subfolders specify the value of Lambda0 (e.g "**D1/**", "**D1e-04/**", etc.). The simulation cases which are then contained within these consist of the same file structure that was already described for

Folder type 1. In the name of the simulation "**..._Mpsi..._**" is however replaced by "**..._MpsiO..._**" to indicate the dilution-enhanced regime.

- The folder "**ExampleSpinoAssistedCryst**" contains additional cases of crystallization in immiscible binary blends. In this case, different Khill, Eps and Kap values were tried out. The simulations presented in the article can be found under "**Khill1p2648/Eps1e-05_Kap1e-10/**". Here, subfolders named only with values of "**Mpsi.../**" contain simulations that are immiscible (+ possibly diffusion-limited, depending on the value of "Mpsi") but not dilution-enhanced. Conversely, the subfolders that read "**MpsiDDep_MpsiO..._D.../**" stand for systems that are immiscible + dilution-enhanced (+ possibly diffusion-limited, depending on the value of "Lambda0").

- The folder "**SingleComponentReference**" provides a reference simulation for a pure component system (i.e. 100% of crystallizable solute material) where only the Allen-Cahn equation is active.

- The folder "**SearchForRepellingCrystals**" contains simulation cases with different surface tension parameter combinations to visualize the tendency of crystals to stick together in clusters or spread over the simulation domain. It was seen that increasing the ratio epsilon/kappa produces crystal grains that tend to avoid clustering and adopt rounder shapes. However, within the range of parameters analysed here, crystals that fully repel each other due to surface tension effects were not achieved. Nevertheless, this could be witnessed in other simulations with different material and thermodynamic parameter sets that also relied on the same code. Effects of increased orientation mismatch energy coefficents were also investigated in the subfolders named "**EpsGrain.../**".

- Finally, the folder "**Eps1e-05_Kap1e-10_Mpsi100/**" contains a preliminary simulation in the regular crystallization regime and with the parameters indicated by the folder's name. Typical simulations can be visualized here without having to parse through the folder structure.

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Folder type 3:

- In the folder "**Article_Figures/**", all final figures used in the different sections of the article and the supplementary information are provided.

The simulations used to produce Fig.3 and Fig.4 (Sec.4.1) are accessible under the "**512x512_dx1e-09/EpsVar/EpsVar_Kap1e-10_Mpsi0p1/Eps1e-05/**" folder path.
For Fig.3-a), the snapshots are taken from the simulation "**CrystInBlend_2D_PCBM-DCB_Mesh512_dx1e-09_T333K_Phi0p4_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-13_5e-10_1e-12_2e-**

09]_Mpsi0p1_Khill0p7248_Khisl1p0836_ACNoise1_CHNoise0".
For Fig.3-b), the snapshots are taken from the simulation "**CrystInBlend_2D_PCBM-DCB_Mesh512_dx1e-09_T333K_Phi0p6_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-13_5e-10_1e-12_2e-09]_Mpsi0p1_Khill0p7248_Khisl1p0836_ACNoise1_CHNoise0**".
For Fig.3-c), the snapshots are taken from the simulation "**CrystInBlend_2D_PCBM-DCB_Mesh512_dx1e-09_T333K_Phi0p8_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-13_5e-10_1e-12_2e-09]_Mpsi0p1_Khill0p7248_Khisl1p0836_ACNoise1_CHNoise0**".
For Fig.4-a) and Fig.4-b), all the simulations within this folder ("**512x512_dx1e-09/EpsVar/EpsVar_Kap1e-10_Mpsi0p1/Eps1e-05/**") are used.

The simulations used to produce Fig.5 (Sec.4.2) and Fig.SI3 (SI-D) are gathered in folders of type 2 (see above for more details).

The simulations used to produce Fig.6 (Sec.5.1) are accessible under the "**512x512_dx1e-09/DVar/Eps1e-05_Kap1e-10_Mpsi0p1/D[1e-19_5e-16_1e-18_2e-15]/**" folder path.
For Fig.6-a), the snapshots are taken from the simulation "**CrystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi0p4_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-19_5e-16_1e-18_2e-15]_Mpsi0p1_Khill0p7248_Khisl1p0836**".
For Fig.6-b), the snapshots are taken from the simulation "**CrystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi0p5_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-19_5e-16_1e-18_2e-15]_Mpsi0p1_Khill0p7248_Khisl1p0836**".

The simulation used to produce Fig.7-a) (Sec.5.1) is accessible under the "**512x512_dx1e-09/DVar/Eps1e-05_Kap1e-10_Mpsi0p1/D[1e-20_5e-17_1e-19_2e-16]/**" folder path.
The name of the simulation is "**CrystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi0p5_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-20_5e-17_1e-19_2e-16]_Mpsi0p1_Khill0p7248_Khisl1p0836**".

The simulation used to produce Fig.7-b) (Sec.5.1) is accessible under the "**512x512_dx1e-09/DVar/Eps1e-05_Kap1e-10_Mpsi0p1/D[1e-22_5e-19_1e-21_2e-18]/**" folder path.
The name of the simulation is "**CrystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi0p5_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-22_5e-19_1e-21_2e-18]_Mpsi0p1_Khill0p7248_Khisl1p0836**".

The simulations used to produce Fig.9 (Sec.5.2) are accessible under the "**512x512_dx1e-09/ExampleSpinoAssistedCryst/Khill1p2648/Eps1e-05_Kap1e-10/Mpsi1000/**" folder path.

For Fig.9-a), the snapshots are taken from the simulation "**CrystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi0p4_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-13_5e-10_1e-12_2e-09]_Mpsi1000_Khill1p2648_Khisl1p0836**".
For Fig.9-b), the snapshots are taken from the simulation "**CrystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi0p6_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-13_5e-10_1e-12_2e-09]_Mpsi1000_Khill1p2648_Khisl1p0836**".

The simulations used to produce Fig.10 (Sec.5.3) are accessible under the "**512x512_dx1e-09/ExampleSpinoAssistedCryst/Khill1p2648/Eps1e-05_Kap1e-10/Mpsi1000000/**" folder path.
For Fig.9-a), the snapshots are taken from the simulation "**CrystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi0p2_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-13_5e-10_1e-12_2e-09]_Mpsi1000000_Khill1p2648_Khisl1p0836**" (in the "**SecondRun/**" subfolder).
For Fig.9-b), the snapshots are taken from the simulation "C**rystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi0p4_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-13_5e-10_1e-12_2e-09]_Mpsi1000000_Khill1p2648_Khisl1p0836**".

The simulations used to produce Fig.11-a) and Fig.11-b) (Sec.5.4) are accessible under the "**512x512_dx1e-09/ExampleMpsiDDep/Eps1e-05_Kap1e-10_MpsiO0p1/D1/**" folder path. All simulations within this folder were used for this figure.

The simulations used to produce Fig.SI4 (SI-E) are accessible under the "**512x512_dx1e-09/DVar/Eps1e-05_Kap1e-10_Mpsi0p1/**" folder path.
For Fig.SI4-a), all simulations within the "**D[1e-19_5e-16_1e-18_2e-15]/**" subfolder were used.
For Fig.SI4-b), all simulations within the "**D[1e-13_5e-10_1e-12_2e-09]/**", "**D[1e-19_5e-16_1e-18_2e-15]/**", "**D[1e-20_5e-17_1e-19_2e-16]/**" and "**D[1e-22_5e-19_1e-21_2e-18]/**" subfolders were used.

The simulations used to produce Fig.SI5 (SI-F) are accessible under the "**512x512_dx1e-09/ExampleSpinoAssistedCryst/Khill1p2648/Eps1e-05_Kap1e-10/Mpsi1000/**" folder path. All simulations within this folder were used for this figure. In addition, the curve from Fig.4-b) of the main article was also used in Fig.SI5-b).

The simulations used to produce Fig.SI6 (SI-G) are accessible under the "**512x512_dx1e-09/ExampleSpinoAssistedCryst/Khill1p2648/Eps1e-05_Kap1e-10/Mpsi1000/**" folder path.
For Fig.SI6-a), the snapshots are taken from the simulation "**CrystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi0p2_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-13_5e-10_1e-12_2e-09]_Mpsi1000_Khill1p2648_Khisl1p0836**".

For Fig.SI6-b), the snapshots are taken from the simulation "**CrystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi0p3_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-13_5e-10_1e-12_2e-09]_Mpsi1000_Khill1p2648_Khisl1p0836**".
For Fig.SI6-c), the snapshots are taken from the simulation "**CrystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi0p5_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-13_5e-10_1e-12_2e-09]_Mpsi1000_Khill1p2648_Khisl1p0836**".
For Fig.SI6-d), the snapshots are taken from the simulation "**CrystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi0p7_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-13_5e-10_1e-12_2e-09]_Mpsi1000_Khill1p2648_Khisl1p0836**".

The simulation used to produce Fig.SI7-a) (SI-H) is accessible under the "**512x512_dx1e-09/ExampleMpsiDDep/Eps1e-05_Kap1e-10_MpsiO0p1/D1/**" folder path.
The name of the simulation is "**CrystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi0p4_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-13_5e-10_1e-12_2e-09]_MpsiO0p1_Khill0p7248_Khisl1p0836**". It is also used in Fig.12 (Sec.5.4) of the main article.

The simulation used to produce Fig.SI7-b) (SI-H) is accessible under the "**512x512_dx1e-09/ExampleMpsiDDep/Eps1e-05_Kap1e-10_MpsiO0p1/D1e-04/**" folder path.
The name of the simulation is "**CrystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi0p4_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-17_5e-14_1e-16_2e-13]_MpsiO0p1_Khill0p7248_Khisl1p0836**". It is also used in Fig.12 (Sec.5.4) of the main article.

The simulation used to produce Fig.SI7-c) (SI-H) is accessible under the "**512x512_dx1e-09/ExampleSpinoAssistedCryst/Khill1p2648/Eps1e-05_Kap1e-10/MpsiDDep_MpsiO0p1_D1e-03/**" folder path.
The name of the simulation is "**CrystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi0p4_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-16_5e-13_1e-15_2e-12]_MpsiO0p1_Khill1p2648_Khisl1p0836**". It is also used in Fig.12 (Sec.5.4) of the main article.

The simulation used to produce Fig.SI7-d) (SI-H) is accessible under the "**512x512_dx1e-09/ExampleSpinoAssistedCryst/Khill1p2648/Eps1e-05_Kap1e-10/MpsiDDep_MpsiO0p1_D1e-04/**" folder path.
The name of the simulation is "**CrystInBlend_2D_PCBM-DCB[N1_5p0298_N2_1]_Mesh512_dx1e-09_T333K_Phi0p4_PowCryst1_Lfus20000_Wfus40322p5806_Eps1e-05_Kap1e-10_D[1e-17_5e-14_1e-16_2e-13]_MpsiO0p1_Khill1p2648_Khisl1p0836**". It is also used in Fig.12 (Sec.5.4) of the main article.