Supporting Information

The Origins of Enhanced and Retarded Crystallization in Nanocomposite Polymers

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Movie 1:
Pure hexacontane (C₆₀H₁₂₂) is being crystallized at T=325K and P=1 atm, during ~56 ns of crystallization time. The movie is made from 600 individual frames, and the point of view is changed by 2 degrees at every frame, allowing for viewing the dynamic process of crystallisation from different angles. Individual molecules are shown with different colours for clarity to observe their conformation and formation of crystal lamella. The simulation includes 61400 united atoms.

Movie 2:
Hexacontane (C₆₀H₁₂₂) gold nanocomposite with a 4.5 nm cubic gold nanoparticle at the centre is crystallized at T=325K and under constant pressure (P=1 atm) for 56 ns. The volume fraction, in this case, is 3.2 %. The simulation includes 87480 hexacontane united atoms and 4794 gold atoms. Individual molecules are shown with different colours for clarity to observe their conformation and formation of crystal lamella. The movie is made from 600 individual frames, and the point of view is changed by 2 degrees at every frame, allowing for viewing the dynamic process of crystallisation from different angles.

Movie 3:
Slices of contours of the final degree of crystallinity (g²) after 56 ns of crystallization of pure hexacontane (C₆₀H₁₂₂). The results are shown at ~0.68 nm intervals in the XZ plane. The red regions have >90% crystallinity, whereas blue regions are amorphous.

Movie 4:
Slices of contours of the final degree of crystallinity (g²) after 56 ns of crystallization of composite gold hexacontane (C₆₀H₁₂₂). The cubic gold particle at the centre is 4.5 nm, and the volume fraction is 2.31 %. The slices are shown at ~0.55 nm intervals in the XZ plane. The red regions have >90% crystallinity, whereas blue regions are amorphous.