Structural and dynamic properties of poly(ethylene oxide)/silica nanocomposites as studied by molecular dynamics simulations: Effects of temperature and silica concentration

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Polymer nanocomposites (PNCs) prepared by introducing nanoparticles (NPs) (spheres, cylinders, plates) within a polymer matrix, have attracted significant scientific and technological interest since the addition of a small volume of nanofillers creates a great amount of interfacial area between polymer matrix and nanofillers, resulting in either improved or new properties without losing attractive properties inherent to pure polymers such as toughness, processability and optical transparency [1]. Molecular dynamics simulation is a complementary tool to experiments as it offers a detailed and direct insight into the properties of a polymer matrix embedded with spherical NPs. Motivated by pertinent experimental and numerical works, we examine structural and dynamic attributes of a poly(ethylene oxide)/silica PNC in a wide range of temperatures sampling both the melt and the glassy state. The effect of NP concentration is also addressed. Our results demonstrate that the dynamics of the adsorbed chains is slower compared to their non-adsorbed counterparts and reveal a coupling between the chain conformational states and their segmental dynamics.
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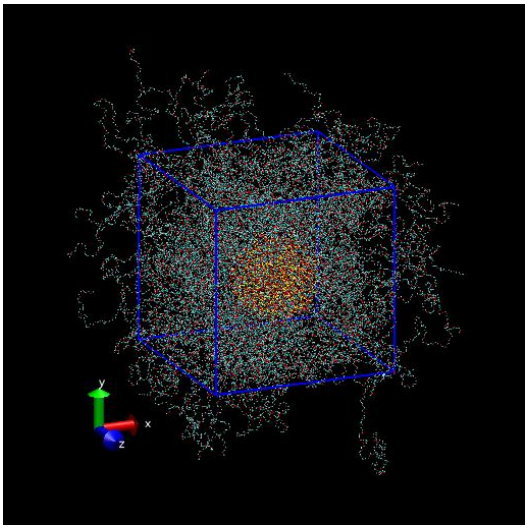

Figure 1: Atomistic representation of the PEO/Silica configuration at silica v / v = 4.5 %.

References

[1] Bailey E.J. and Winey K.I., Progress in Polymer Science, **105** 101242 (2020).

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