MOLECULAR MECHANICS SIMULATION OF ALUMINOSILICATE NANOTUBES (IMOGOLITE): MECHANICAL RESPONSE UNDER COMPRESSION AND PROPERTIES WHEN THE NANOTUBE IS IMMERSED IN WATER

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The control of the morphology of nanoparticles is the daily work of many researchers around the world. Imogolite was discovered in the late 1960s in volcanic soils and, in 1977 a protocol for their synthesis was published. The chemical formula of imogolite is \((\text{Al}_2\text{SiO}_7\text{H}_4)_{2N}\), with \(N = 10\) in the natural case and \(N = 11-15\) for the synthetic one. This clay nanotube (NT) has the characteristic of having an effective control of its diameter during the synthesis and based on experimental evidence, imogolite nanotubes are highly monodisperse in diameter regardless of the diverse synthesis conditions.

The mechanical response of aluminosilicate nanotubes (imogolite) under compression is investigated by means of classical molecular dynamics simulations using the CLAYFF potential. Using the uncompressed length \(L_0\), when there is no strain, to describe each nanotube, we have found that imogolite tends to coil for \(L_0 > 15\) nm to prevent the failure of the nanotube. The simulation also shows that the nanotubes do not break under stress for \(L_0 > 100\) nm. Finally, we can report a Young modulus of the order of 200 GPa.

Also, in this contribution, simulations for imogolite immersed in water are presented. This system is studied using Classical Molecular Dynamics Simulations (MD) with LAMMPS and Grand Canonical Monte Carlo (GCMC) simulations. Both employ CLAYFF force field and SPC water model. GCMC is used to obtain the water density in the inner pore of the imogolite at 300 K. This obtained water density is included in the MD simulations of imogolite NTs immersed in water. Periodic boundary conditions along the axis of the NT are considered in the NVT ensemble at 300 K. The simulation analysis includes (i) one-dimensional (1D in radial direction) water density profiles form the center of the NT and (ii) two-dimensional (2D) water density profiles and (iii) water diffusion close to the imogolite. During the simulations, the imogolite with \(N = 8\) is found highly hydrophobic meanwhile for \(N > 10\) the water is well ordered in the inner pore of the NT.

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