

ORGANO-VERMICULITE STRUCTURE ORDERING AFTER PVAC INTRODUCTION: EXPERIMENT AND MODELING

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Interactions of clay minerals with organic polymers have increasing interest from the industrial and scientific perspectives. Layered silicates, in particular clay minerals, have been used because their excellent intercalation abilities.

Natural clays, containing inorganic cation in interlayer, are hydrophilic, while exchanging an inorganic cation to certain large organic cation, the clay properties are altered and material becomes hydrophobic.

The role of surfactant molecules is to prepare more opened organophilic host material with larger interlayer spacing. The alkyl ammonium ions of surfactant are cationic exchanged for the inorganic cations in clays, a lateral bilayer or inclined paraffin-like structure results. At higher concentration of onium ions a lipid-like structure is formed [1]. This organo-clay readily accepts other neutral molecules. The combination of a nano-dimensional clay material with a polymer may yield either a microcomposite, in which the clay is acting as filler and is not dispersed at the nanometer level, or a true nanocomposite. Though vinyl acetate is water-soluble, there is not required an organophilicity of vermiculite; organo-vermiculite assured suitable space for monomer sorption and polymerization.

Simulation techniques become an essential adjunct to experimental techniques, since the information about the spatial arrangement of molecules within the interlayer is hard to obtain without the aid of computer simulation [2, 3].

In this study were observed:

- Changes of vermiculite interlayer space after intercalation with different quaternary ammonium salts using X-ray diffraction method.
- Changes of organo-vermiculite structure after introduction of monomer and following polymerization Fig.1.
- Molecular interaction of individual components in the modified vermiculite and nanocomposite using IR spectroscopy.
- Simulation possibilities for the nanocomposite systems Fig.2.

References:

- [1] N.A.D'Souza in: H.S.Nalwa (Ed.) Encyclopedia of Nanoscience and Nanotechnology 3, Am. Sci. Publishers, 2004 253-265
- [2] R.Toth, A.Coslanich, M.Ferrone, M.Fermeglia, S.Priol, S.Miertus, E.Chiellini, Polymer **45** (2004) 8075.
- [3] K.S.Katti , D.Sikdar, D.R.Katti, P.Ghosh, D.Verma, Polymer **47** (2006) 403.

Figures:

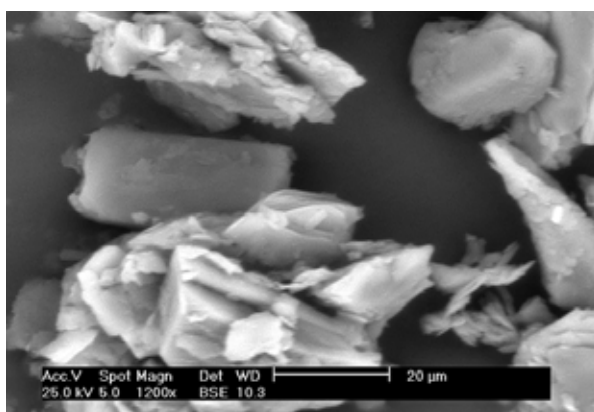


Fig.1 Scanning electron microscopy image of nanocomposite

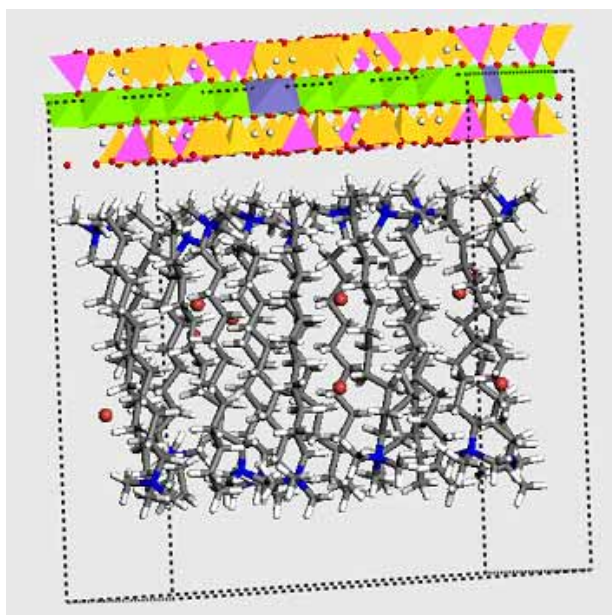


Fig.2 Structure of organo-vermiculite simulated using *MS Accelrys*