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Measurement and correlation of PVT for organic-inorganic hybrid nanoparticles

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Abstract (less than 300 words)

Organic-inorganic hybrid nanoparticles (HNPs), which are composed of inorganic core nanoparticles and organic surface modifiers, have been expected to be used as fillers in polymer functional materials. HNPs are usually single-nanometer in size and their behaviors in polymer materials have been occasionally recognized as those of molecules as well as solids. This might be attributed to the small size of HNPs.

In our research, we have attempted to apply molecular thermodynamics to the HNPs. The features of surface modifiers and core parts are quite different, and it is very important to characterize quantitatively their influence on properties. One possible method for the functional evaluation of HNPs is PVT measurement. However, there have been reported no data and useful approaches in the literature.

In this work, carboxylic acid-modified ceria nanoparticles are adopted as a model HNP. The PVT was measured with the bellows type apparatus originally developed by Y. Sato *et al*^[1]. The validity of the experimental apparatus and procedure were firstly demonstrated by measuring the PVT of decane. The obtained experimental PVT data were correlated with the Tait equation^[2] and the Sanchez-Lacombe equation of state (S-L EoS)^[3], which are widely applied to thermodynamic property calculations of polymer systems. PVT measurement data indicated that the specific volume increases with increasing temperature and decreases with increasing pressure. Such PVT behaviors were well correlated with the above equations. In correlating with S-L EoS, the EoS parameters were determined by assuming the HNP as a pseudomolecules and the density reflects the contributions of core and surface modifier.

References

- [1] Y. Sato et al., J. Appl. Polym. Sci., 66, 141 (1997)
- [2] P. G. Tait, Voyage of H. M. S. Challenger, 2, 1 (1989).
- [3] I. C. Sanchez and R. H. Lacombe, J. Phys. Chem., 80, 2352 (1976).

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