Computational modelling of graphite exfoliation in shear flow by using immersed finite element method

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ABSTRACT

Flow-based exfoliation of graphite is a good candidate in developing a mass production method of high-quality graphene. Unfortunately, the hydrodynamic force is not sufficient to exfoliate single-layer graphene from bulk graphite due to van der Waals (vdW) forces acting on graphene layers. In this case, intercalants are inserted between the graphene layers for widening the interlayer gap size. After the intercalation, the exfoliation of graphite by shear flow is possible. However, the direct measurement of the exfoliation process in situ is still challenging in state-of-the-art experimental techniques. So it is essential to find an alternative way of predicting the exfoliation process. In this talk, a computational method is suggested to predict the exfoliation process of graphene layers in shear flow. For developing the method, the chemical intercalation was simulated by quantum calculation and molecular dynamics. From the simulation result, the vdW force acting on the interlayer was estimated as a multi-scaling parameter for simulating fluid-structure interaction between intercalated graphene layers and fluid flow. The fluid-structure interaction is simulated by an immersed finite element method with mass-spring model. Finally, the exfoliation process of graphene layers in shear flow is predicted by the simulation. In addition, critical shear rates in various intercalation conditions will be fully discussed during the presentation.

REFERENCES

[1] Tuan Sang Tran, Seung Jun Park, Sung Sic Yoo, Tae-Rin Lee, TaeYoung Kim, "High shear-induced exfoliation of graphite into high quality graphene by Taylor–Couette flow", *RSC Advances*, Vol. **6**, pp. 12003-12008, (2016).