Testing our Understanding of the Shear Exfoliation Model

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In 2008 it was discovered that graphite could be delaminated in liquid media using sonic energy and stabilized in monolayer and few layer forms through use of appropriate solvents.[1] Sonication is a high energy process, requiring expensive equipment and the process does not scale well to large scale production volumes. This was addressed in 2014 when Paton et al. demonstrated exfoliation of graphene to monolayer using high shear mixing.[2]

Figure 1 Silverson high shear mixer used for production of graphene in [2]

As a relatively new technique, shear mixing raised many questions as the process differs significantly from sonication. It was found, for example, that exfoliation did not occur below a certain range of shear rate (~ 10^4 s^{-1}). Applying a simple model, considering the exfoliation as shear-induced inter-layer sliding in solvent, yielded an equation giving the minimum shear rate as:

$$\dot{\gamma}_{\min} = \frac{[\sqrt{E_{S,G}} - \sqrt{E_{S,L}}]^2}{\eta L}$$

However this equation predicts much more than simply the presence of a minimum shear rate for exfoliation and this work seeks to test this equation. For example controlling flake size for a given solvent through variation of applied shear rate or minimizing the shear needed to exfoliate through appropriate solvent choice.

In this work the exfoliation behavior of shear mixing is tested and compared to earlier surface energy studies tested on graphite. The shear exfoliation model is then tested using two other 2D layered materials, MoS_2 and WS_2, and minimum shear rate for exfoliation is demonstrated for both of these materials. Finally through absorption spectra metrics from[3] flake length and thickness can be easily measured for dispersions of MoS_2. This is then plotted as a function of applied shear rate.

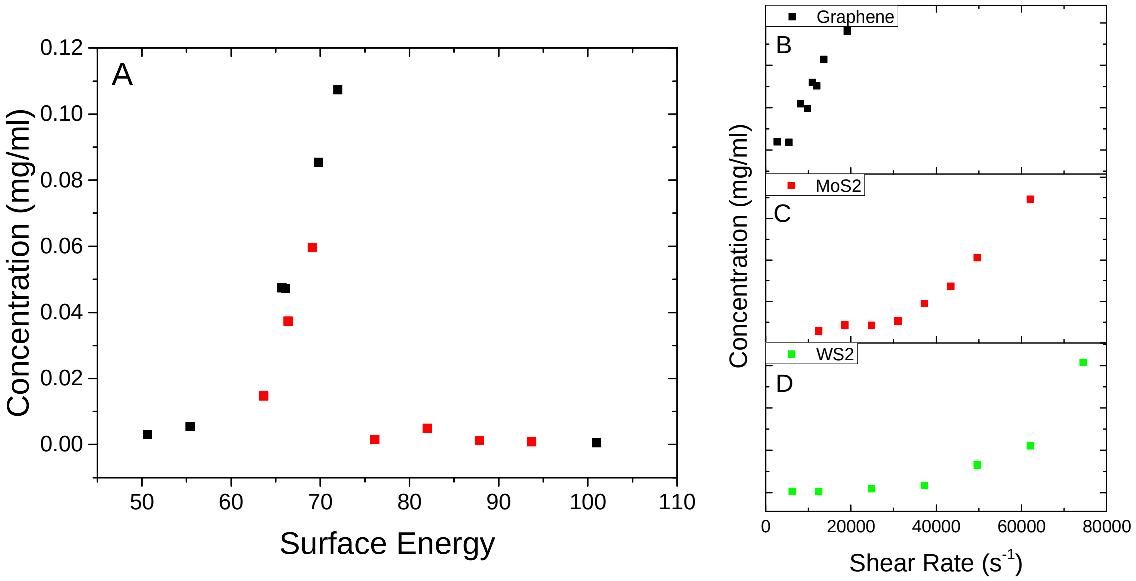

Figure 2: (A) Plotting dispersed concentration as a function of surface energy (B-D) Demonstrating shear min for various materials

The simple shear model is found to be remarkably accurate at predicting the behavior of sheared dispersions and is found to be broadly applicable to a 3 separate materials, demonstrating that it is not specific to graphite. Flake size effects are observed for all 3 materials, indicating a potential method of flake size control. Some difficulties in separating the variables exist however making it difficult to test the model completely.

References

1. Hernandez, Y., et al., Nat. Nanotechnol., 2008. **3**: p. 563.
2. Paton, K.R., et al., *Scalable production of large quantities of defect-free few-layer graphene by shear exfoliation in liquids.* Nat Mater, 2014. **13**(6): p. 624-630.
3. Backes, C., et al., *Edge and confinement effects allow in situ measurement of size and thickness of liquid-exfoliated nanosheets.* Nat Commun, 2014. **5**.
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