Abstract

In this work, we present an empirical approach to nanoscale titanium diboride (TiB_2), a layered ceramic from the metal diboride family. We have developed this approach by integrating co-solvency with the surface tension component matching theory. It is gradually being established that layered metal diborides can be exfoliated in a liquid phase to yield 2D counterparts. However, these reports have not yet systematically investigated the suitability of a solvent to exfoliate these ionic layered materials. Such a prospect is primarily limited by the fact that the theories available to rationally select exfoliating solvents are applicable only for van der Waals (vdW) layered materials. We show that it is possible to identify an optimal exfoliating medium for TiB_2 by using co-solvents. In the approach that we developed, we first test the exfoliation of TiB_2 in isopropanol (IPA)-water co-solvent mixtures at different IPA concentrations. This enables us to practically observe exfoliation of TiB_2 at a range of P/D values (ratio of polar and dispersive surface tension components), by using only two solvents mixed at varied proportions. We used this simple approach to identify the P/D value at which exfoliation of TiB_2 was optimal (~1.1). We could also show that this resultant P/D value serves as a guiding point to predict the fate of TiB_2 in other solvents. TiB_2 did not exfoliate efficiently in acetonitrile ($P/D \approx 2.2$) but exfoliated well in glycerol ($P/D \approx 1.2$). Furthermore, the nanosheets obtained by this approach are found to be minimally functionalized - the original structural integrity of nanosheets (TiB_2 lattice) is maintained to a large extent after exfoliation. Such a minimal functionalization led us to observe moiré patterns for the first time in the nanosheets of this family. These near pristine nanosheets present a curious construct to assess how a planar confinement in these nanostructures would affect the properties of TiB_2. It would be promising to test this approach on other members of layered metal diborides (like MgB_2 and AlB_2), as well as other ionic layered materials.

Keywords: Layered metal diborides, two-dimensional (2D) nanostructures, titanium diboride (TiB_2), borophene, liquid-phase exfoliation, surface tension components, and co-solvents.