Structure and physicochemical properties of MgB2 nanosheets obtained via sonochemical liquid phase exfoliation

(Article begins on next page)

18 October 2024

SUPPLEMENTARY INFORMATION

Structure and physicochemical properties of MgB$_2$ nanosheets obtained via sonochemical liquid phase exfoliation

Santanu Kumar Padhi[1], Xiaolin Liu[2], Maria Carmen Valsania[3], Luca Andreo[3], Angelo Agostino[3], Andrea Alessio[1], Linda Pastero[4], Alessia Giordana[3], Zhilin Wu[2], Giancarlo Cravotto[2], Marco Truccato[1,*]

[1] NIS Interdepartmental Centre and Physics Dept. University of Torino, Via P. Giuria 1, 10125 Torino, Italy

[2] Drugs Dept. University of Torino, Via P. Giuria 9, 10125 Torino, Italy

[3] NIS Interdepartmental Centre and Chemistry Dept. University of Torino, Via P. Giuria 7, 10125 Torino, Italy

[4] NIS Interdepartmental Centre and Earth Science Dept. University of Torino, Via Valperga Caluso 35, 10125 Torino, Italy

*Corresponding author: marco.truccato@unito.it
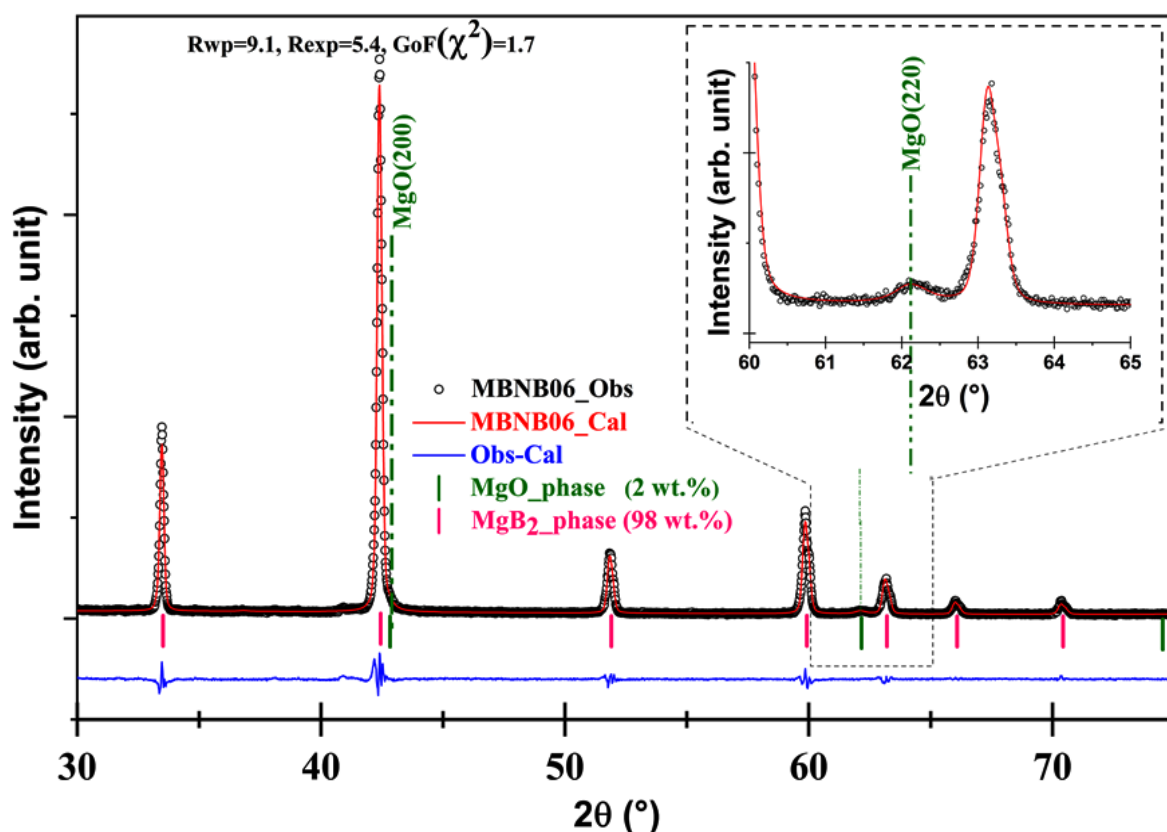
Figure S1: Representative XRD pattern of MgB_2 sample obtained with Mg:B = 1.4:2 at T=800°C and coded as MBNB06. Black void circles represent experimental observed data points, red solid line is the calculated best fit via the Rietveld refinement method, and the solid blue line at the bottom is the corresponding residual. The expected Bragg positions of the peaks are labelled by vertical solid ticks in olive (MgO) and pink (MgB_2) colours, respectively. A zoomed portion of this XRD pattern from 60-75° is included as an inset highlighting the MgO(220) well-resolved peak position.

The sample's X-ray diffraction (XRD) pattern was acquired with a Philips X'Pert diffractometer (PW3040/60 X'Pert PRO model). The absolute scan mode data acquisition for a 2θ range between 30° and 75° was carried out with a step size of 0.02°. The Rietveld refinement was performed using the MAUD (Material Analysis Using Diffraction) program [1,2]. The crystal structure input data was obtained from the Inorganic Crystal Structure Database, ICSD (for MgB_2: ICSD database code 96706, and for MgO: ICSD database code 52026). The percentage weight fractions (wt. %) of the different crystalline phases resulting from the refinement procedure, along with the standard R-factor values (i.e., the weighted profile R-factor R_{wp}, the expected R-factor R_{exp}, and GoF(χ^2) =R_{wp}/R_{exp}, respectively) characterizing the quality of the fit have been inserted as text in Fig.S1.
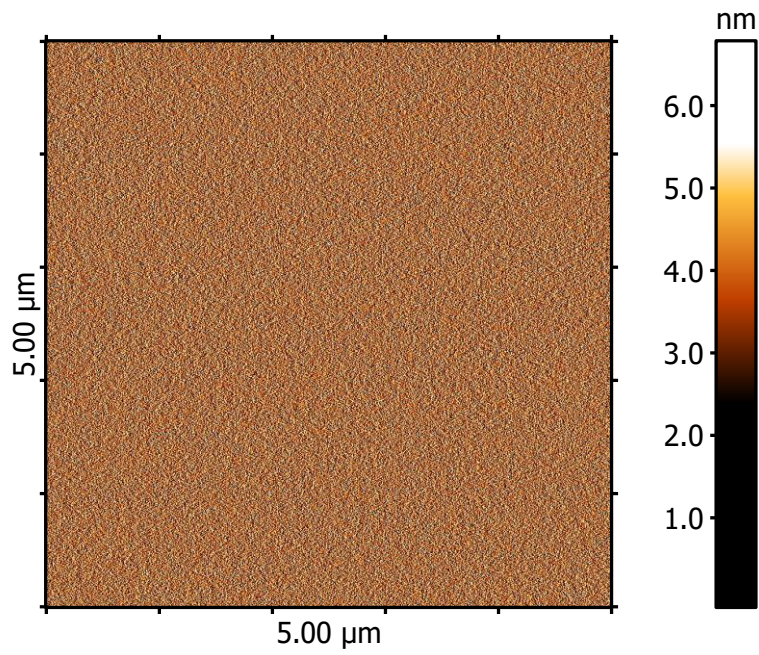
**Figure S2**: STM topographic map of a typical sapphire substrate coated with 20 nm Au, measured before the deposition of MgB_2 nanoparticles via drop-casting. The coated surface shows an rms roughness $S_{rms} = 0.58$ nm.
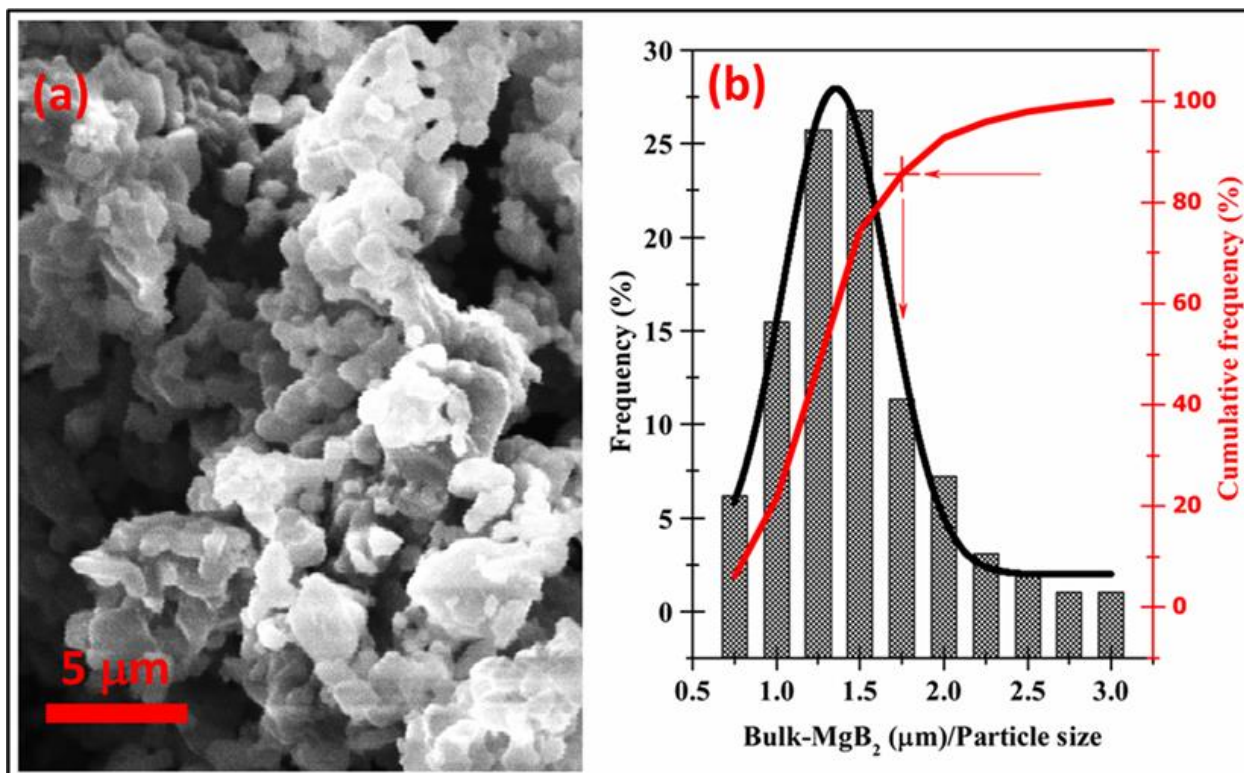
Figure S3: SEM observation of the precursor MgB_2 powder used to produce the sonicated suspensions. (a) secondary electron micrograph indicating hexagonal-plate particle morphology; (b) corresponding histogram for the particle size distribution. The black curve represents a fit to a gaussian curve of the experimental distribution (mean size = 1.4 ± 0.4 μm). The red curve is the cumulative distribution function.

Fig.S3(a) displays a SEM micrograph of the precursor MgB_2 powder that underwent the sonication treatments. It can be noticed that the material consists of many small grains with a typical shape of hexagonal-like platelets. The histogram of their size distribution is reported in Fig.S3(b): the mean grain size is 1.4 ± 0.4 μm and more than 85 % of the particles show a size less than 1.8 μm.
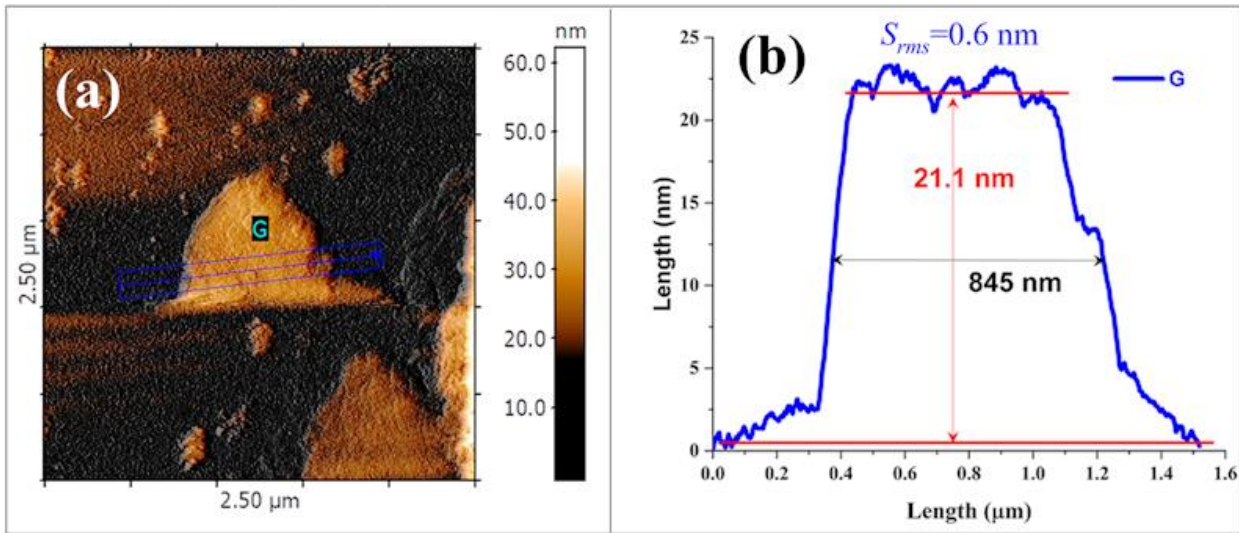
Figure S4: (a) STM topographic map for an example of extended nanosheet observed in the 1h sonicated suspension. (b) Profile of the nanosheet measured along the blue line indicated in panel (a). Width of the sheet is equal to 845 nm, average height is 21.1 nm and the rms roughness is $S_{rms} = 0.6$ nm, which is approximately equal to the one of the bare substrate ($S_{rms} = 0.58$ nm). For this nanosheet the width-to-height ratio is approximately equal to 40.

References

1. Lutterotti L, Matthies S, Wenk HR. MAUD (material analysis using diffraction): a user friendly Java program for Rietveld texture analysis and more. In: *Proceeding of the Twelfth International Conference on Textures of Materials (ICOTOM-12)*. Vol 1. NRC Research Press Ottowa, Canada; 1999:1599.

2. Lutterotti L. Total pattern fitting for the combined size–strain–stress–texture determination in thin film diffraction. *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*. 2010;268(3):334-340. doi:10.1016/j.nimb.2009.09.053