2D materials such as MoS$_2$ and graphene are ideal candidates for developing novel nanocomposites with improved properties for the transport industry. A challenge to overcome for polymer matrix composites manufacture is to obtain high homogeneity filler dispersion within the matrix. Imaging simulation techniques can help us to explore the limits of characterizing bidimensional structures with only a few atoms at atom-scale and facilitate a correct interpretation of molecular studies performed by novel electron microscopes. However, when the composition of the filler and polymer matrices are similar, in terms of average atomic number, as it is the case of graphene, the structural characterization of these composites using Scanning Transmission Electron Microscopy (STEM) imaging techniques is hard. We show in this communication, based on STEM image simulations, that this technique can be helpful to know the dispersion of fillers in amorphous matrices.

In relation to filled-graphene nanocomposites, our study based on simulation techniques and structure-modeling images shows the possibility of functionalizing graphene layers with gold atoms to enable their location in a carbon matrix by Z-contrast STEM. Firstly several atomic models representing graphene composites marked with gold atoms and surrounded by amorphous carbon were built (fig.1A-B). Secondly, high-angle annular dark-field (HAADF) STEM images of these specimens were simulated by applying the multislice algorithm using SICSTEM [Pizarro et Al. Appl. Phys. Lett. 93, 153107 (2008)] and analyzed. All simulations were performed using CAI supercomputer [http://supercomputacion.uca.es].

Results ensure that unmarked graphene simulated images present a homogeneous contrast, making impossible to distinguish where the graphene sheets are placed in an amorphous material representing the matrix of a polymer-based nanocomposite. However, when the graphene sheet orientation coincides with the beam orientation of the microscope, the position of unmarked graphene can be clearly detected inside the amorphous matrix because of the channeling effect. Furthermore, the results demonstrate that marking graphene sheet with individual gold atoms allows identifying and locating graphene in reinforced amorphous areas, regardless of their spatial orientation (fig.1C). Finally, it has been observed that the focal series simulations enable us to know the optimum focus.

Regarding MoS$_2$, due to the high atomic number of molybdenum, it is not necessary to mark the layers with heavier atoms to localize them within the matrix. Nevertheless, it is worth to explore the limits of detectability of HAADF-STEM, so we are currently simulating different configurations and orientations of these layers within an amorphous carbon matrix.

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Fig. 1: A) Isolated graphene sheet viewed from [100] direction marked with gold nanoparticles. B) Complete model dimensions: 8x4x8nm of amorphous carbon (blue) encircling a parallel graphene sheet (green), which is marked with tree gold nanoparticles (red). C) HAADF image. D) Intensity values at optimum focus represented on a surface with model dimension.