Amorphous carbon and amorphous materials in general are of particular importance for high resolution electron microscopy, either for bulk materials, generally covered with an amorphous layer when prepared by ion milling techniques, or for nanoscale objects deposited on amorphous substrates. In order to quantify the information of the high resolution images at the atomic scale, a structural modeling of the sample is necessary prior to the calculation of the electron wave function propagation. It is thus essential to be able to reproduce the carbon structure as close as possible to the real one. The approach we propose here is to simulate a realistic carbon from an energetic model based on the tight-binding approximation in order to reproduce the important structural properties of amorphous carbon.

In this work, we propose a new method to model in a more realistic way amorphous carbon (a-C) that accurately accounts for its 3D structure. It is based on an energetic approach with a tight-binding (TB) potential in which the electronic band structure of the material is calculated with the recursion technique. The main advantage of this model is that it gives a very good description of the sp, sp2, and sp3 hybrid bonds and their competition [1].

At first, the model and the main structural properties of the generated carbon will be presented and compared with a simple model of carbon, where the atom positions are generated randomly. We have shown that the limit thickness for the wave phase approximation is 30% overestimated if we consider the random carbon model (Fig. 1). In a second step, we have studied the influence of the carbon model on the contrast of single Cu, Ag and Au atoms deposited on amorphous carbon substrate. Our work does not indicate any significant influence of the carbon structure on single-atom contrast when statistically relevant measurements are performed. Finally, we have compared both model structures for the determination of the long-range order parameter in a small CoPt nanoparticles deposited on a-C layer. We have clearly shown the importance to use realistic amorphous carbon model to obtain quantitative values for the diffracted intensities. As it can be observed on Figure 2, diffuse scattering intensity due to the 3D atomic arrangements of the realistic carbon has a significant contribution to the scattered information especially at low spatial frequencies [1].

This work emphasizes the necessity to use realistic carbon model for TEM image and diffraction simulation in order to extract very sensitive quantitative information, particularly in diffraction experiments.


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Fig. 1: Comparison of the (a) phase and (b) intensity of the transmitted beam (i.e., the unscattered part of the electron wave) calculated using Random and tight-binding carbon structures as a function of the thickness layer. The slice thickness is 0.25 nm. The simulation box size in the layer plane is 5nx5 nm with a 1024x1024 sampling.

Fig. 2: Electron diffraction calculation of a CoPt NP with a LRO of 0.4 deposited on a 10 nm thick amorphous carbon layer simulated by (a) the random model and (b) the tight-binding model. (c) Radially integrated intensity profile as a function of the scattering vector for both diffraction patterns (a) and (b) in black and red, respectively.