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Graphene-covered iron layers on Ni(111): structural and electronic properties HELIO CHACHAM, SABRINA S. CARARA, GUILHERME J. P. ABREU, ROBERTO PANIAGO, EDMAR A. SOARES, Universidade Federal de Minas Gerais, Brazil — Recently, Dekdov et al. [Appl. Phys. Lett. 93, 022509 (2008)] reported the intercalation of atomic Fe layers between graphene and a Ni surface. In the present work, we report new experimental and theoretical results on this novel nanostructure. Fe intercalation was produced by repeatedly evaporating monolayers of ^{57}Fe on previously prepared graphene/Ni(111), and post-annealing at 320 C. In situ Mössbauer spectra are consistent with a single hyperfine magnetic field for the one-Fe-monolayer system, while the two- monolayer system presented two field values. By using low energy electron diffraction (LEED) the strucuture of both graphene/Ni(111) and graphene/Fe/Ni(111) was investigated. The model that best fits the experimental LEED curves corresponds to one C atom on top of Ni or Fe and the other C atom on a fcc hollow-site, consistent with the most stable systems in the first-principles calculations. Regarding the calculated electronic structure of the studied systems, the graphene/Ni structure presents a bandgap of 0.06 eV for the minority-spin electronic states near the original graphene Fermi point. The inclusion of Fe layers modify the magnitude, and even the existence, of such bandgap. For instance, in the case of the one-Fe-monolayer system, the bandgap increases to 0.63 eV.

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