DFT studies of Graphene on Ni(111) and Surface Nickel Carbide Ni$_2$C ANDREAS GARHOFER, Vienna University of Vienna, PETER JACOBSEN, Vienna University of Vienna, Tulane University, BERNHARD STÖGER, GARETH S. PARKINSON, MICHAEL SCHMID, Vienna University of Vienna, ROMAN CAUDILLO, Intel Corporation, FLORIAN MITTENDORFER, JOSEF REDINGER, Vienna University of Vienna, ULRIKE DIEBOLD, Vienna University of Vienna, Tulane University — Graphene with its unique transport properties supported on ferromagnetic materials is a promising candidate for the fabrication of spin-filtering devices. In order to study the growth of graphene on metal surfaces, graphene on Ni(111) is a perfect system from a structural point of view. The CVD growth of graphene on Ni(111) was studied with STM. The experiments showed not only perfect aligned (1x1) structures, but also several moiré patterns are observed. They are due to grain rotations of graphene on both Ni(111) and also surface nickel carbide Ni$_2$C. During CVD growth carbon atoms segregate into the Ni bulk. With an increasing carbon concentration first the surface carbide and then a graphene layer on top is built. We studied the systems using the DFT program package VASP with the DFT-D2 method of Grimme to include van der Waals interactions. In our theoretical analysis we tried to understand the formation of the graphene and Ni$_2$C on Ni(111). We calculated the stability of the surface carbide phase and the binding energies of rotated and unrotated graphene on Ni(111) as well as on Ni$_2$C in order to understand the experimental findings. Graphene and Ni$_2$C have no epitaxial relationship due to their incommensurate lattices, leading to a spread in grain rotations.

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