MD simulations of hydrogen plasma interaction with graphene surfaces DAVID GRAVES, University of California at Berkeley, EMILIE DESPIAU-PUJO, ALEXANDRA DAVYDOVA, GILLES CUNGE, CNRS/UJF-Grenoble1/CEA LTM, LAURENCE MAGAUD, CNRS/UJF-Grenoble 1 Institut Néel — Development of graphene-based technologies relies on the capability to grow and integrate this new material into sophisticated devices but the nm-scale control of graphene processing challenges current processing technology. Plasma-graphene interactions must be carefully controlled to avoid damage to the active layers of graphene-based nanoelectronic devices. Pulsed plasmas will minimize surface damage from ions, and help control neutral chemistry, but they must be better understood. We applied molecular dynamics (MD) simulations, coupled with experiments, to better understand and control the plasma-graphene surface interaction. The influence of graphene temperature and incident species energy on adsorption, reflection and penetration mechanisms is presented. Except for impacts at graphene nanoribbon edges or at defects location, H species are shown to experience a repulsive force due to delocalized $\pi$-electrons which prevents any species with less than $\sim 0.6$eV to adsorb on the graphene surface. Bonding of H to C requires a local rehybridization from sp2 to sp3 resulting in structural changes of the graphene sample. Energetic H+ bombardment of stacked multilayer graphene sheets are analyzed and the possibility to store hydrogen between adjacent layers is discussed.

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