Energetics and structure of FeO/Fe(001) interfaces

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Thin FeO layers on bcc iron surfaces play an important role in early stages of iron surface oxidation, oxides growth, corrosion, magnetic devices and spintronics. We present results of DFT study of interaction of FeO(001) atomic layers with Fe(001) surface. It is found that adsorption of FeO monolayer on the Fe(001) surface results in a surface covered by oxygen atoms and a growth of subsequent oxide layers at the surface precovered by oxygen. For films of 2–6 FeO(001) monolayers thick on Fe(001) surface, the system with oxygen atoms at the FeO/Fe(001) interface is energetically most stable. The deposited FeO(001) films affect weakly the geometry of the Fe(001) surface, causing small expansion of the first interlayer distance compared to the clean iron surface. The calculated adhesion energies show that the strongest FeO-Fe(001) interaction occurs for a triple FeO layer film, which is by more than 2.0 eV stronger bound to Fe(001) surface than the FeO monolayer. For thicker FeO films (4-5 layers of FeO) the interaction weakens, however it remains stronger than for the FeO monolayer film. It is also found that FeO(001) films on Fe(001) surface exhibit antiferromagnetic ordering.