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**Atomistic modeling of surface alloy formation for Fe deposited onto flat and stepped Pt substrates** CARY PINT, Department of Physics and Astronomy, Rice University, GUILLERMO BOZZOLO, NASA Glenn Research Center/Ohio Aerospace Institute, JORGE GARCES, Centro Atomico Bariliche, Argentina — Fe-Pt alloys are of significant importance toward applications of high-density magnetic recording media. In this work, we apply the BFS method for alloys to study the energetic pathway for subsurface Fe-Pt alloy formation upon deposition of Fe atoms on (flat) Pt(100), Pt(111), and (stepped) vicinal Pt(997) substrates. We observe the preference for Fe atoms to decorate Pt step edges upon Fe deposition on Pt(997), allowing the formation of an ordered Fe-Pt surface alloy at the edges of the monatomic surface steps with increasing thermal energy. Compared to the formation of a surface alloy from deposition on a low-index Pt surface, we observe that step decoration of the Fe atoms on Pt(997) reduces the strain energy required for Fe surface penetration, resulting in a lower energy barrier associated with the formation of an Fe-Pt subsurface alloy. The results are found to be in agreement with experiment, and the formation of the Fe-Pt subsurface alloy in each case is explained by a simple analysis emerging from the competition between BFS strain and chemical energy contributions.

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