

THEORETICAL STUDY OF FECO/W(110) SURFACE ALLOYS

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Using first-principles band-structure theory we have calculated structural and magnetic properties of two-dimensional FeCo ordered alloys deposited on W(110) substrate. For pseudomorphic overlayers a decrease of the total magnetic moment with increasing Co content has been found in agreement with experimental observation of decreasing Curie temperature. In a homogeneous Co/W(110) overlayer the ferromagnetic, $c(2 \times 2)$ antiferromagnetic and nonmagnetic solutions are virtually degenerated. We show that an extraordinary strong Co–W interaction is responsible for the reduction of magnetism in the Co overlayer. In addition, an experimentally observed non-pseudomorphic close-packed overlayer with 10 Co atoms placed over every 8 W atoms along the [100] direction has been explored. The surface structure with an incomplete dislocation is found to be favored over the structure containing a complete misfit dislocation. The close-packed Co overlayers are ferromagnetic.