Perpendicular Magnetic Anisotropy of Ultratin FeCo Alloy Films on Pd(001) Surface

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Using the full potential linearized augmented plane wave (FLAPW) method, thickness dependent magnetic anisotropy of ultrathin FeCo alloy films in the range of 1 monolayer (ML) to 5ML coverage on Pd(0 01) surface has been explored. We have found that the FeCo alloy films have close to half metallic state and well-known surface enhancement in thin film magnetism is observed in Fe atom, whereas the Co has rather stable magnetic moment. However, the largest magnetic moment in Fe and Co is found at 1ML thickness. Interestingly, it has been observed that the interface magnetic moments of Fe and Co are almost the same as those of surface elements. The similar trend exists in orbital magnetic moment. This indicates that the strong hybridization between interface FeCo alloy and Pd gives rise to the large magnetic moment. Theoretically calculated magnetic anisotropy shows that the 1ML FeCo alloy has in-plane magnetization, but the spin reorientation transition (SRT) from in-plane to perpendicular

Magnetization is observed above 2 ML thickness with huge magnetic anisotropy energy. The maximum magnetic anisotropy energy for perpendicular magnetization is as large as 0.3 meV/atom at 3 ML film thickness with saturation magnetization of 2.36 µB. Besides, the calculated X-ray magnetic circular dichroism (XMCD) has been presented.

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