SF-P005

A first principles study on magnetism of Fe3Si on Si(001) and Si(111) substrates

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The current interest in transition metal-semiconductor heterojunctions arises from fundamental and technological issues. For applications in magnetoelectronics/spintronics the main focus is on the ferromagnetic (FM) metallic films which can be grown epitaxially on most common semiconductors. A well defined Fe_3Si thin film can be synthesized on Si, because of the similar crystal structure and the small lattice mismatch (-4%). Using the full-potential linearized augmented plane wave (FLAPW) method within general gradient approximation (GGA), we have studied the electronic structure and magnetic properties of the FM Heusler alloy Fe_3Si on Si(001) and Si(111) substrates as well as Fe_3Si(111) surface, which have recently been grown by molecular-beam epitaxy (MBE). We focus on the surface and interface effects on the magnetism and have taken into account all possible surface terminations including relaxations of these surfaces. The magnetic moments at the surfaces considered in this study are much enhanced compared to those of the corresponding bulk due to surface effect. Especially, the calculated magnetic moment ($2.78\mu_B$) of Fe(II)-terminated system of Fe_3Si(111) surface is significantly enhanced two times than the bulk value. The surface DOS of Fe_3Si(111) and Fe_3Si on Si(111) showed them to be "*nearly*" half-metallic, dissimilar to the bulk one.

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SF-P006

Magnetism and magnetocrystalline anisotropy of Fe monolayer on W substrates: A first principles study

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Transition metal (TM) thin films exhibit significantly different magnetic behavior depending on surface crystallographic orientation of the nonmagnetic substrates. The magnetic ordering of 3*d* TM monolayer (ML) on the bcc W substrate is an example. An Mn ML on W(001) surface becomes ferromagnetic (FM) while there are antiferromagnets on W(110) surfaces. In contrast to Co and Fe ML on W substrate show opposite magnetic behavior. The atomic numbers of the TM and nonmagnetic substrates play a key role in determining the magnetic behavior. Although this systems has been studied extensively in the past, the magnetic anisotropy of Fe films on W substrates have not been studied in detail theoretically yet. In this work, we investigated magnetism and magnetocrystalline anisotropy (MCA) of the Fe ML on W(001) and W(110) surfaces. The calculations were performed using the highly precise full-potential linearized augmented plane-wave (FLAPW) method within general gradient approximation (GGA) for exchange correlation potential. We simulated the system as a single slap which consists of Fe ML attached on each side of seven-layers of W. The experimental bcc W lattice constant a = 3.16 Å was used. From total energy calculation, an antiferromagnetic (AFM) state was found to be energetically more stable, compared to a FM states for Fe ML on W(001) surface. On the contrary, Fe ML on W(110) surface was found be a FM state. Detailed discussion on the correlation between unusual magnetism and MCA will be discussed.

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