DFT study for ferromagnetic thin film of iron siliside on Si(111) surface

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SiFe on Si(111) is considered as one of the most ideal device material for ecological point of view. The structure of the thin film SiFe on Si(111) surface is investigated by Walter et.al. using DFT calculation. [1] However, recently, K.Hattori et.al. i[2,3] reported that the SiFe thin layers on Si(111) has ferromagnetic behavior. Previous calculation by Walter et.al. did not comment on the magnetic properties of their several structure models in their work. The very recent experiments study magnetism of the SiFe/Si(111) surfaces[2], They prepared high quality samples in ultra-high vacuum and carried out in-situ LEED, RHEED, STM, SMOKE and ex-situ SQUID measurements. These implies that the Si(111)1x1- and 2x2-Fe surfaces are super-paramagnetic and ferromagnetic, respectively, and that the ferromagnetic moment arises from the c-FeSi(111) film or the interface. Therefore, we investigate here the magnetic properties of the several known models of SiFe/Si(111) using DFT calculation. The total-energy and electronic-structure calculations are performed using the DFT calculation with LDA and GGA. We expand the electronic wave functions into plane waves up to an energy cutoff of 30 Ry. The result shows us that the so-called 6Layers-A5 and 6Layers-B5 structures[1] are the candidate of the structure of SiFe/Si(111). "B" means the B-type stacking[1]. The A5 and B5 are stable than the other structures using the total energy analysis due to the DFT calculation. We also found that only A5 and B5 show spontaneous spin polarization. It agrees with the experiments that the SiFe/Si(111) has ferromagnetic behavior. The origin of the spin polarization is the Fe atoms of the interface layer, not surface layer. We also confirm that the bulk structure of SiFe has no magnetic behavior. According to the calculation and related experiments, the ferromagnetic behavior appears only for few layers of SiFe thin films. Therefore, we can conclude that the structure of the SiFe thin layers on Si(111) is A5 or B5 structure.

References

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