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Theoretical Investigation of the Metallic Spacer-Layer Formation of Fe/Si Multilayered Films

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Abstract

We have carried out the first-principle electronic structure calculations to investigate the spacer layer formation of Fe/Si multilayered films (MLF) and compared with the results obtained by optical spectroscopy. The computer-simulated spectra based on various structural models of MLF showed that neither $FeSi_2$ nor *B*20-phase FeSi, which are semiconducting, could be considered as the spacer layers in the Fe/Si MLF for the strong antiferromagnetic coupling. The optical properties of the spacer extracted from the effective optical response of the MLF strongly support its metallic nature. The optical conductivity spectra of various phases of Fe-Si compounds were calculated and compared with the extracted optical properties of the spacer. From the above theoretical investigations it is concluded that a *B*2-phase metallic FeSi compound is spontaneously formed at the interfaces during deposition.

1. Introduction

After a strong antiferromagnetic (AF) coupling in Fe/Si multilayered films (MLF) was discovered [1,2], there were numerous studies to elucidate the characteristics of the spacer layer. It was controversial whether the spacer layer for a strong AF coupling between ferromagnetic layers of Fe/Si MLF was metallic or semiconducting. The reactive Fe/Si interface formation mechanism and the resulting interface structure appear to be problems of intriguing complexity. It is quite well known that the metastable crystalline *B*2-phase FeSi is responsible for a strong AF coupling between Fe sublayers in the Fe/Si MLF. We already provided some supporting information on the structure and stoichiometry of the spacer layer in Fe/Si MLF extensively applying the optical and magneto-optic (MO) spectroscopies [3]. The main idea of Ref. [3] is based on the fact that in a metallic MLF structure the reflected light carries information on the near surface layer of a few tens of nm thick. The optical response from the MLF is directly related to the optical properties of the constituent layers and depends on the structural parameters of the MLF, such as thickness and stoichiometry of the constituent sublayers, interfacial mixing, roughness of the interface, and so on, in a complex way.

It was concluded that the metastable crystalline *B*2-phase FeSi is spontaneously formed in the interfacial regions of the Fe/Si MLF by using the experimental, computer-simulated MO and optical spectroscopies. In this paper we report our new theoretical results of the first-principles calculations to confirm the experimental results.

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2. Details of Theoretical Calculations

We employed the scalar-relativistic version of the tight-binding linear-muffin-tin-orbital method within the local-density approximation and the local-spin-density approximation for the paramagnetic and the ferromagnetic phases, respectively. An atomic-sphere approximation was employed and the combined-correction term was included. The spin-orbit interactions were included in a perturbative way. We calculated the electronic structures for several different stoichiometries, such as Fe_3Si, Fe_2Si, Fe_5Si_3, and *B*2-phase FeSi. For the equiatomic FeSi we calculated the electronic structure only for the *B*2-phase since the *B*20-phase FeSi is a small-gap semiconductor (see below). The lattice constants are 20.15 Å (Fe_2Si), 20.196 Å (Fe_3Si), 24.123 Å (Fe_5Si_3), and 9.892 Å (FeSi). Note that Fe_3Si, Fe_2Si and Fe_5Si_3 alloys have more than one formula unit in a conventional unit cell.

3. Results and Discussion

The experimental results of magnetic, optical and MO properties are presented in Ref. [3]. We will discuss the optical conductivity [$\sigma(\omega)$] spectra only. The $\sigma(\omega)$ spectrum of the (3.0 nm Fe/1.8 nm $Si)_{50}$ MLF (solid circle) is displayed in Fig. 1 together with Si (open circles), amorphous FeSi2 (down solid triangles), and ε-FeSi (solid squares). Two kinds of spacer layers were employed in the simulations. The simulation method is explained in Ref. [3] in detail. The dashed and solid lines represent the extracted $\sigma(\omega)$ spectra for the spacers whose stoichiometries are FeSi and Fe_5Si_3, respectively. The structure of the interfacial regions which are spontaneously formed during the deposition of the Fe/Si MLF depends on the nominal sublayer thickness. In contrast to the Fe/Si MLF with relatively thick sublayers, an amorphous structure with a short-range order close to the semiconducting *B*20-phase FeSi (or β-$FeSi_2$) structure is spontaneously formed in the Fe/Si MLF with sublayers

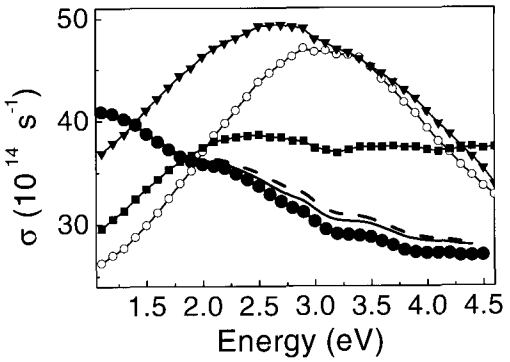

Fig. 1. Various optical conductivity [$\sigma(\omega)$] spectra for the (3.0 nm Fe / 1.8 nm Si)50 MLF.

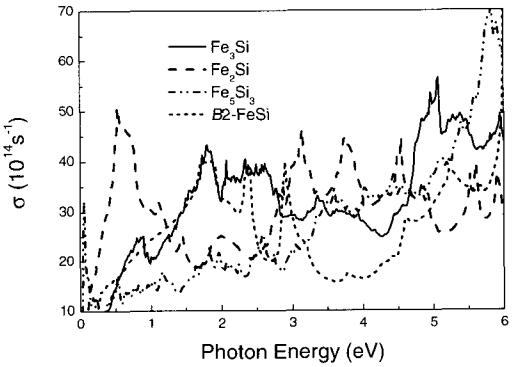

Fig. 2. Calculated optical conductivity spectra for various iron silicides.

thinner than 1 nm [3]. However, these MLF with thin sublayers do not exhibit strong AF coupling. This result strongly suggests that the spacer layer with a metallic character mediate the AF coupling. Previous experimental investigations [4,5] also concluded that a strong AF coupling in Fe/Si MLF was mediated by the spacer layer with a metallic character. As can be seen in Fig. 1, the extracted spectra closely resemble to the experimental one when the spacer layer is either FeSi or Fe_5Si_3. To check these results we calculated the spectra for the iron silicides with various stoichiometries.

Fig. 2 presents the calculated spectra for Fe_3Si, Fe_2Si, Fe_5Si_3, and *B*2-phase FeSi. We did not include the *B*20-phase FeSi, which is more stable in bulk phase, because it is a strongly correlated small-gap

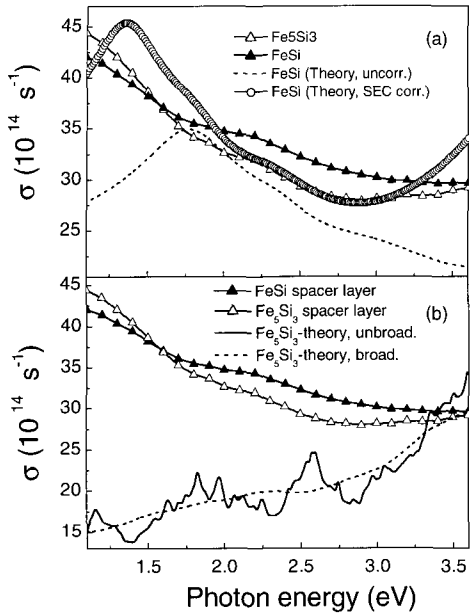

Fig. 3. Experimentally extracted $\sigma(\omega)$ spectra of the spacer for the *B*2-phase FeSi and Fe_5Si_3 stoichiometries together with calculated and broadened $\sigma(\omega)$ spectra for(a) FeSi and (b) Fe_5Si_3 alloys.

semiconductor. Therefore, neither Si, nor *B*20-phase FeSi can be considered as the spacer layer mediating the strong AF coupling. It should be noted here that only Fe_2Si and *B*2-phase FeSi alloys are possible candidate for the spacer layer since they have the spectra exhibiting decreasing magnitude of $\sigma(\omega)$ with increasing energy in the 1.0-4.5 eV range. If the Si sublayer is completely consumed during the deposition, forming iron silicide, the stoichiometry is not very off to the equiatomic one and thus the Fe2Si is excluded for the further consideration as the spacer for the AF coupling.

In Fig. 3 the extracted $\sigma(\omega)$ spectra were compared with the calculated ones using the first-principles. From Fig. 3(b) the Fe_5Si_3 alloys can be excluded although it is metallic. The metallic *B*2-phase FeSi is the most suitable for the spacer layer. Since the calculated and broadened $\sigma(\omega)$ spectrum for *B*2-phase FeSi resembles the experimentally extracted $\sigma(\omega)$ spectra except the peak positions, we applied the real part of the self-energy correction (SEC), or λ-fitting, to match their energy positions [see Fig. 3(a)].

4. Conclusions

The optical properties of the spacer layer for the AF coupling in the Fe/Si MLF were extracted, which strongly supports its metallic nature. This fact allows us to suggest that the AF coupling in the Fe/Si MLF is mediated by the metallic spacer. We have calculated the spectra for the iron silicides with various stoichiometries. Among them the *B*2-phase FeSi and the Mg_5Si_3-type Fe_5Si_3 alloys were considered as the spacer layer for the AF coupling. The experimentally extracted spectra of the silicide spacer that mediates a strong AF coupling in the Fe/Si MLF with relatively thick sublayers strongly suggest that the spacer is a metallic FeSi silicide.

Acknowledgements

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