Striped - honeycomb transition of domain wall structure of ^{3}He submonolayer solid film on graphite

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Abstract

We predict the striped (superheavy) - honeycomb (heavy) structural phase transition of the domain wall structure of ^{3}He submonolayer solid film on a graphite surface at 6.8 nm^{-2} based on the adsorption energy calculation by the path integral Monte Carlo simulation. The experimentally observed sudden jump of the Debye temperature at the same density can be explained by this transition within the multiple spin exchange model.

Key words: ^{3}He film; adsorption structure; multiple spin exchange

1. Introduction

The magnetism of ^{3}He solid film adsorbed on a graphite surface is determined by the competition of the multiple spin exchange (MSE) interactions [1,2]. It has become clear that the MSE competition is strongly affected by the corrugation of adsorption potential [3–5]. This fact should mean that it is necessary to clarify the adsorption structure in order to understand the magnetism of adsorbed ^{3}He solid film. Unfortunately, it is difficult to observe directly the adsorption structure of ^{3}He film on graphite by some experimental reasons. In the recent publication we propose a structural phase diagram of the submonolayer solid film on graphite, which can explain experimental observations quantitatively, based on the path integral Monte Carlo simulations [5]. In that consideration we omitted the rather low areal density regime. In this paper we report the results of the calculations of the adsorption energy for some plausible domain wall structures there. These are rather preliminary but show the possible structural transition between the striped domain wall structures and the honeycomb ones.

2. Calculation and discussion

In the adsorbed system on graphite the domain wall structures are thought to appear at slightly higher areal density of the $\sqrt{3}\times\sqrt{3}$ structure, 6.4 nm^{-2}. Also in the ^{3}He and ^{4}He films on graphite such domain wall structures are predicted but have not observed yet [6,7]. The adsorption energies per ^{3}He atom are calculated for the heavy striped domain wall (SDW), superheavy SDW and heavy honeycomb domain wall (HDW) structures with some periodicity by the path integral Monte Carlo method with the periodic boundary condition. These structures are schematically shown in Fig. 1(a)-(c), respectively. The results are shown in Fig. 2. The energies of 'honeycomb cage' structures [5] are also shown. It clearly shows that the heavy SDW structure is unstable all over the areal density range. Unfortunately at the lower areal density region the calculation consumes so much time because the unit cell is so large, and the calculation is not enough now. However, the result seems to show that while above 6.8 nm^{-2} the heavy HDW structure is most stable, below this density the superheavy SDW is more stable. That is, the striped - honeycomb transition of the domain wall structure should occur at around 6.8 nm^{-2}. Similar evolution has been

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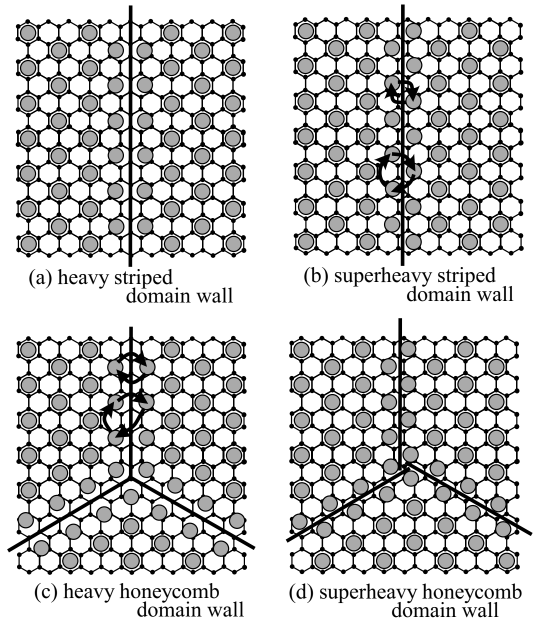

Fig. 1. Some plausible adsorption structures are schematically shown. The grey circles show the position of ^{3}He atoms, and small honeycomb shows the graphite lattice. The solid lines indicate the domain wall. Some atomic exchange paths are also shown by arrows.

observed in the D_2 film [8].

The Weiss temperature θ of ^{3}He film obtained in the magnetization measurements has a jump at around this density [3]. Below this density θ is almost constant and positive (ferromagnetic). While, above this density θ has small absolute value or negative value (antiferromagnetic). In the heavy domain wall the 3-spin exchange path makes a right-angled triangle with a long side and two acute angles as shown with arrows in Fig. 1(c). That should be unfavorable to the 3-spin exchange, which produces the ferromagnetic interaction. For the 2-spin exchange, which produces the antiferromagnetic interaction, hindrances by the neighboring atoms should be weaker than in the triangle lattice or in the superheavy wall. These facts should mean that the ferromagnetic interaction is suppressed by the SDW - HDW transition, i.e., by the superheavy - heavy transition. This tendency agrees with the experimental observation. In the $\sqrt{3}\times\sqrt{3}$ phase the potential corrugation suppresses the 2-spin exchange stronger than the 3-spin exchange [3,4]. By the SDW - HDW transition the area occupied by the $\sqrt{3}\times\sqrt{3}$ structure is reduced. That may also be responsible to the sudden magnetic change. We cannot conclude whether the phase transition is the first order or second order within the accuracy of our calculation. However, if the jump of θ is due to the structural transition that must be the second order phase transition. The melting temperature

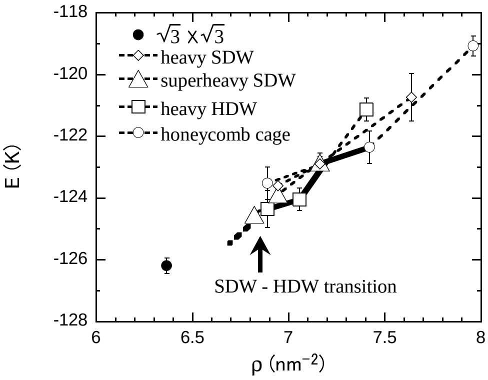

Fig. 2. The calculated adsorption energies per ^{3}He atom for some adsorption structures.

observed in the heat capacity measurements also seems to have a weak kink at this density [9]. The structural phase transition can be responsible to such a change.

Although the superheavy HDW as shown in Fig. 1(d) seems unstable, the existence of such structure cannot be excluded now. Also the other possible structures must be considered.

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