Available online at www.sciencedirect.com
ScienceDirect
Surface Science 601 (2007) 1642–1645
SURFACE SCIENCE
www.elsevier.com/locate/susc

Transformation to soluble model for structural phase transition from (4×1) to $(8 \times$ "2") of In-adsorbed Si(1 1 1) surface

Yoichiro Yagi [a,*], Akio Yoshimori [a,1], Kiminori Kakitani [b], Hiroko Kaji [b]

[a] Department of Computer Simulation, Okayama University of Science, 1-1, Ridai-cho, Okayama 700-0005, Japan
[b] Department of Electronic Engineering, Okayama University of Science, 1-1, Ridai-cho, Okayama 700-0005, Japan

Received 22 December 2006; accepted for publication 31 January 2007
Available online 4 February 2007

Abstract

The Ising model proposed previously for the structural phase transition from (4×1) to $(8 \times$ "2") of In-adsorbed Si(1 1 1) surface, Hamiltonian of which is consisting of a two-spin interaction as well as a four-spin interaction is shown to be equivalent in thermodynamic properties to a soluble Ising model with two-spin interactions. Temperature dependence of the long range order and the transition temperature can now be determined from the exact formulae. Comparison between the simulation results and those from the exact formulae is made to see accuracy of the simulation.

Keywords: Ising models; Monte Carlo simulation; LEED; Scanning tunneling microscopy; X-ray scattering, diffraction, and reflection; Surface thermodynamics (including phase transitions); Indium; Silicon

1. Introduction

The structural phase transition from (4×1) to $(8 \times$ "2"), with decreasing temperature, of In-adsorbed Si(1 1 1) surface is explained by the Ising model with a two-spin as well as a four-spin interaction, which we previously proposed [1]. Many experimental and theoretical investigations on this phase transition have been made [2–23]. Interesting aspects of this transition may be summarized as follows; it is the second order phase transition but the ordered phase still has some disorder shown by diffuse half-order spots in X-ray and electron diffraction down to liquid helium temperatures [1,7,13].

This highly anisotropic system consists of two zigzag In chains in the (4×1) unit cells along the b-axis ($4a$ and b are fundamental translational vectors, whose details are explained in the next section), which show a quasi-one-dimensionality to some extent. (In this paper, the two zigzag In chains in the (4×1) unit cells along the b-axis are called simply the (4×1) chains.) The Pierls mechanism of the In zigzag chain seemingly contributes to doubling of unit cell along the b-axis and the short range order, which originates from the mechanism, starts at pretty higher temperatures. Each zigzag In chain has two ways of doubling and the two zigzag chains can have four ways of independent doubling by symmetry. In the low temperature phase, a coupling between neighboring (4×1) chains along a-axis allows only two out of the four doublings and those two different in the neighboring (4×1) chains. Those allowed two are degenerate by symmetry and produce disorder observed in the diffraction experiments. This is indeed the reason why the low temperature phase is described by $(8 \times$ "2"). (To be precise, it should be (8×1) as used by Ref. [13].)

In this paper, we first show by a rather simple nonlinear transformation on Ising spins that our previous model is equivalent in thermodynamic properties to a soluble Ising model with anisotropic two-spin interactions on a rectangular lattice and, then, we have the exact formulae for

* Corresponding author. Tel./fax: +81 86 256 9653.
E-mail address: yagi@sp.ous.ac.jp (Y. Yagi).
[1] Present address: 2-20-15-402, Shinsenri-kitamachi, Toyonaka, Osaka 560-0081, Japan.

0039-6028/$ - see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.susc.2007.01.047

many physical quantities. We compare the temperature dependence of the long range order parameter and the transition temperature from those formulae with the results by the previous Monte Carlo simulation to know its accuracy for an extended model, we are going to take in the forth-coming publication.

This paper is constructed as follows. In the next section, our Ising model with two- and four-spin interactions on the rectangular lattice, whose unit cell contains two-spins, is transformed into an Ising model with two-spin interactions on a Bravais rectangular lattice. In Section 3, temperature dependence of the long range order parameter and the transition temperature from the exact formulae are compared with the results obtained previously and also newly by the Monte Carlo simulation. Section 4 concludes the paper with summary and discussions for the present results and ongoing further works.

2. Transformation from two- and four-spin interaction model to two-spin interaction model

Our previous model was given by the Hamiltonian, H

$$H = J\sum_{lmv}\mu_{lmv}\mu_{l,m+1,v} + K\sum_{lm}(\mu_{lm0}\mu_{lm1}\mu_{l+1,m0}\mu_{l+1,m1} + \mu_{lm0}\mu_{l,m-1,1}\mu_{l+1,m0}\mu_{l+1,m-1,1}), \quad (1)$$

where J ($J>0$) is the coupling constant between the nearest neighbor pair along the b-axis (we took the rectangular unit cell for (4×1), where $a=(4,2)$ and $b=(0,1)$ on the triangular lattice of Si(1 1 1) surface), μ_{lmv} ($v=0,1$) is Ising spin in the (l,m)th unit cell and K ($K>0$) is the coupling constant for four-spin interaction along the a-axis. It is discussed in Ref. [1] why those interactions are chosen. (In suffix, comma is omitted if it is clear as $l,m,v\rightarrow lmv$.) Those Ising spins, $\mu_{lmv}(v=0,1)$ are local order parameters describing the phase transition.

When we introduce the combined Ising spin S_{lmv} by the following nonlinear transformation,

$$S_{lm0}=\mu_{lm0}\mu_{l,m-1,1},\quad S_{lm1}=\mu_{lm0}\mu_{lm1}, \quad (2)$$

and we notice $\mu_{lmv}^2=1$, we can have the first term of H rewritten as

$$\mu_{lm0}\mu_{l,m+1,0}\mu_{lm1}^2+\mu_{l,m-1,1}\mu_{lm1}\mu_{lm0}^2=S_{lm1}S_{l,m+1,0}+S_{lm0}S_{lm1}. \quad (3)$$

Then, applying the transformation given by Eq. (2) to the second term of H, we have, together with Eq. (3),

$$H = J\sum_{lm}(S_{lm1}S_{l,m+1,0}+S_{lm0}S_{lm1}) + K\sum_{lm}(S_{lm1}S_{l+1,m1}+S_{lm0}S_{l+1,m0}). \quad (4)$$

This Hamiltonian is nothing but the one of the soluble two-dimensional Ising model with the nearest neighbor interaction along each the a- and b-axis on the rectangular lattice, where the lattice point is specified along the b-axis as $(lm0)$, $(lm1)$, $(l,m+1,0)$, $(l,m+1,1)\ldots$, as is shown in Fig. 1.

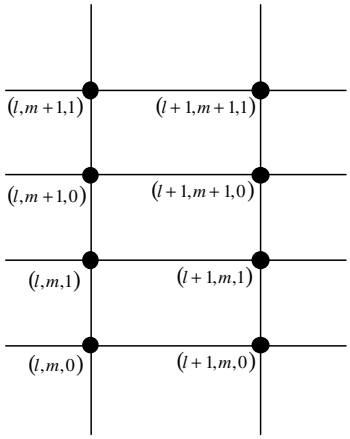

Fig. 1. The rectangular lattice for the transformed Hamiltonian of S-spins.

Important aspect of this transformation, Eq. (2) is that S-spin is defined by the bi-product of μ-spins. Its natural consequence is that the S-spins are invariant under the transformation, $\mu\rightarrow-\mu$ so that H is also invariant (μ represents all μ_{lmv}). This means that each (4×1) chain can have either configuration of μ or $-\mu$ in our model, that is, $\mu_0=1$, $\mu_1=1$ and $\mu_0=-1$, $\mu_1=-1$ for $S_0=1$ as well as $\mu_0=-1$, $\mu_1=1$ and $\mu_0=1$, $\mu_1=-1$ for $S_0=-1$ (common suffices l, m are omitted for simplicity). This accounts for the disorder mentioned in the introduction as is discussed in our previous letter [1]. Then, the S-spins can describe thermodynamic properties but, in order to describe detailed configuration and the disorder in the real system, we need naturally the μ-spins.

It should be noted here that consistency of the boundary conditions along the b-axis on the μ-spins and S-spins needs some caution, although it does not affect the thermodynamic properties even if they are inconsistent. If we employ the free end boundary condition for a finite system, there is perfect consistency by taking $2N_b$ of the μ-spins i.e. μ_{lmv} ($m=1,\ldots N_b$, $v=0,1$) and $2N_b-1$ of the S-spins i.e. S_{lmv} ($m=1,\ldots N_b-1$, $v=0$, 1 and $m=N_b$, $v=0$) for given l. In this way, degrees of freedom of the μ- and S-spins agree each other by considering the degeneracy of $\mu\rightarrow-\mu$.

If one insists the periodic boundary condition for both the finite spin systems, then number of spins should be the same and there should be strong constraint for the S-spin configurations to kill abundant degrees of freedom. A half of the all possible configurations of the S-spins do not correspond to any possible configurations of the μ-spins and must be discarded.

3. Temperature dependence of the long range order

As we describe in the next section, we are going on to an extended model where the Monte Carlo method is used. It will be useful to know accuracy of the Monte Carlo method on size of the system (including the boundary condition