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Energetics of highly kinked steps edges

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We have determined the step edge free energy, the step edge stiffness and dimensionless inverse step edge stiffness of the highly kinked <010> oriented step on a (001) surface of a simple square lattice within the framework of a solid-on-solid model. We have found an exact expression for the step edge free energy in the case that only nearest neighbour interactions are taken into account. At low temperatures the dimensionless inverse step edge stiffness reduces to the universal value $^1/_2\sqrt{2}$. However, with increasing temperature the dimensionless inverse step edge stiffness increases. Incorporation of an attractive next-nearest neighbour interaction leads to a suppression of the dimensionless inverse step edge stiffness. For a non-zero next-nearest neighbour interaction the dimensionless inverse step edge stiffness even vanishes at zero temperature.

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1. Introduction

Surface steps play a crucial role in many surface processes, such as crystal growth, phase transitions, surface mass transport, thermal roughening and etching [1]. For instance the thermal roughening of a facet of a crystal is determined by the step edge free energy. At the roughening temperature the surface roughens due to vanishing of the step edge free energy. At zero temperature surface steps tend to be as straight as possible since the creation of additional step edge length, i.e. kinks, costs energy. The term 'kink' was introduced by Kossel and simultaneously by Stranski, who referred to a kink as a half crystal position. At non-zero temperatures an increase in the total step edge energy due to kink generation is counteracted by an increase in the step edge entropy. Since the latter term scales linearly with temperature there is even a temperature where the total step free energy becomes zero leading to an unlimited growth of the step edge length. Other examples where the energetics of surface steps play a leading role are for instance faceting and step bunching [2,3]. In these cases not only the step free energy is important, but also the energetic interaction between the steps should be taken into account.

For <110> oriented steps on a simple square (001) lattice no kinks are present at zero temperature. From a statistical mechanical point of view it is rather easy to derive expressions for the step edge free energy, step edge stiffness and the dimensionless inverse step edge stiffness [4–9]. The step edge stiffness is a quantitative measure of the resistance of a step against meandering.

In contrast, a <010> oriented step edge is 100% kinked at zero temperature and therefore it is much more difficult to describe this step in terms of a statistical mechanical framework. Interestingly, in the case that only nearest neighbour interactions are present, <010> oriented steps can meander without the need to create additional step edge length. This leads for low temperatures to a universal (and non-zero) dimensionless inverse step edge stiffness of $^1/_2\sqrt{2}$ [10]. This universal behaviour is, however, destroyed when next-nearest neighbour interactions are taken into account. In the literature several expressions for the dimensionless inverse step edge stiffness have been published that only depend on the next-nearest neighbour interaction and not on the nearest neighbour interaction. As we will show later these expressions describe the low temperature situation rather well, but at elevated temperature they become inaccurate. A statistical mechanical approach to derive, within the framework of a solid-on-solid model, expressions for the step free energy, step edge stiffness and dimensionless inverse step edge stiffness is very appealing since the strength of the nearest neighbour and next-nearest neighbour interactions can be determined experimentally by an analysis of the step edge roughness [11–13]. In the case that only nearest neighbour interactions are considered exact expressions for the step free energy and step edge stiffness can be derived [14]. However, the incorporation of next-nearest neighbour interactions leads to approximate expressions that are only accurate for weak next-nearest neighbour interactions [15,16].

It is the aim of the present paper to derive expressions for the step edge stiffness and dimensionless inverse step edge stiffness that are accurate for temperatures up to a substantial fraction of the roughening temperature. A careful analysis of the meandering of a <010> oriented step edge reveals that the dimensionless inverse step edge stiffness depends on the next-nearest neighbour as well as nearest neighbour interactions. For a non-zero next-nearest neighbour interaction the dimensionless inverse step edge stiffness even vanishes at zero temperature. At elevated temperature the

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dimensionless inverse step edge stiffness increases with increasing temperature.

We will start with the derivation of an expression for the step edge free energy of a 100% kinked <010> oriented step (see Fig. 1(A)). We assume isotropic nearest neighbour (ε_{NN}) and next-nearest neighbour (ε_{NNN}) interactions between the surface atoms. In Fig. 1(B) a schematic diagram of a <010> oriented step edge is shown. In order to determine the step edge free energy it is sufficient to consider an elementary step edge segment of length $a_{//} = {}^1\!/_2\sqrt{2}a$, where a is the surface lattice constant. The partition sum, $Z_{<010>}$, of this elementary step edge segment is given by [4,21],

$$Z_{<010>} = \sum_i e^{-E_i/k_BT} = AB + \sum_{n=0}^{\infty} (AB)^{2n}\left(AB^2 + A^3B^3\right) = \frac{AB(1+B)}{1-(AB)^2} \tag{1}$$

where E_i is the energy of the step edge configuration, k_B is the Boltzmann's constant, T the temperature, $A = e^{-\varepsilon_{NN}/2k_BT}$ and $B = e^{-\varepsilon_{NNN}/2k_BT}$.

The step edge free energy per unit step edge length measured in the <010> direction is,

$$F_{<010>} = -\sqrt{2}k_BT\ln\left[Z_{<010>}\right] = -\sqrt{2}k_BT\ln\left[\frac{AB(1+B)}{1-(AB)^2}\right]. \tag{2}$$

The factor of $\sqrt{2}$ comes from the fact that we have expressed the step edge free energy per unit length a rather than per unit length $a_{//} = {}^1\!/_2\sqrt{2}a$.

In the case that we are only dealing with nearest neighbour interaction (i.e. $B=1$) the step free energy per unit length reduces to,

$$F_{<010>} = -\sqrt{2}k_BT\ln\left[\frac{2A}{1-A^2}\right] = \sqrt{2}k_BT\ln\left[\sinh\left(\frac{\varepsilon_{NN}}{2k_BT}\right)\right]. \tag{3}$$

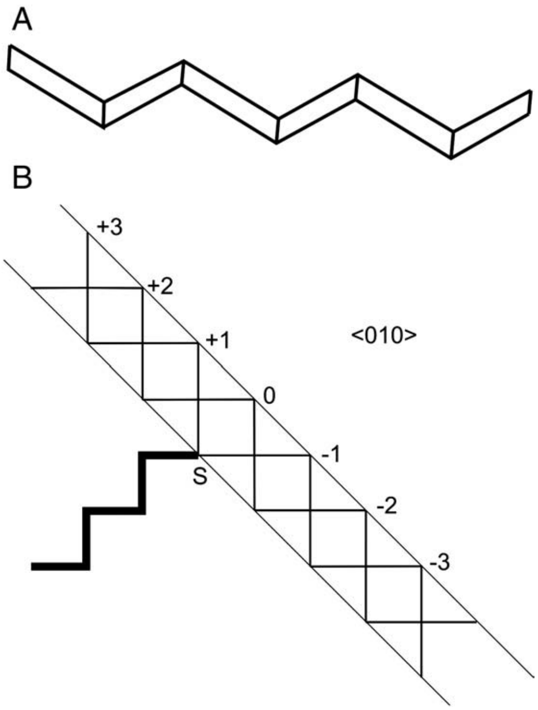

Fig. 1. (A) Schematic 3D view of a <010> oriented step on a (001) surface of a simple square lattice (B) Schematic diagram of a <010> oriented step on a (001) surface of a simple square lattice. The thick solid line is a <010> oriented step. The thin lines refer to possible pathways to make an elementary step $a_{//} = \sqrt{2}a$ in the <010> direction. The labels $0, \pm 1, \pm 2, \ldots$ refer to the kink lengths, which are measured in units of $a_\perp = \sqrt{2}a$.

But this is precisely the exact expression for the interface boundary tension along the <010> direction for the 2D Ising model as derived by Onsager [8,14,17]. This gives us confidence that we have considered all possible step edge configurations. Moreover the step edge free energy of <110> and <010> oriented steps vanishes at exactly the same temperature as one should expect from a physical point of view [8,14,17,18].

After having derived an expression for the step edge free energy we will derive an expression for the dimensionless inverse step edge stiffness. The meandering of a step can be characterized by the spatial step correlation function $G(x)$, which is defined as [19,20],

$$G(x) = <[y(x+x_0)-y(x_0)]^2> = <n^2>\frac{|x|}{a_{//}} \tag{4}$$

where x and y are coordinates parallel and perpendicular to the mean step edge direction, while $a_{//}$ and $a_\perp$ are the atomic units along and perpendicular to the step edge. Finally, $<n^2>$ is the mean-square kink length and is defined as,

$$<n^2> = \sum_i n_i^2 p_i \tag{5}$$

where p_i refers to the probability of finding a kink with a length of $n_i a_\perp$. The summation runs over all possible kink configurations. The mean-square kink length is the expectation value of the square kink length at each step edge position and can be considered as the diffusivity of the step edge. At zero temperature (or infinity large kink creation energy) the step edge diffusivity or mean-square kink length is reduced to zero for a <110> oriented step. But for a <010> oriented the mean-square kink length can have a non-zero value at zero temperature. The spatial step correlation function can also be written in terms of the step edge stiffness $\tilde{\gamma}$ [19,20],

$$G(x) = <[y(x+x_0)-y(x_0)]^2> = \frac{k_BT}{\tilde{\gamma}a_{//}}a_{//}|x| \tag{6}$$

where the dimensionless inverse step edge stiffness is defined as,

$$\frac{k_BT}{\tilde{\gamma}a_{//}}. \tag{7}$$

Thus the following relation between the step edge stiffness and mean-square kink length exists,

$$\frac{k_BT}{\tilde{\gamma}a_{//}} = \frac{<n^2>}{a_{//}^2}. \tag{8}$$

The calculation of the mean-square length is a little cumbersome, but in principle straightforward. By using Eqs. (1) and (5) we find (see Appendix),

$$\frac{k_BT}{\tilde{\gamma}a} = \sqrt{2}\left[\frac{\left(B+A^2B^2\right)\left(1+A^2B^2\right)}{(1+B)\left(1-A^2B^2\right)^2}\right]. \tag{9}$$

Eq. (9) can be written in terms of the nearest and next-nearest neighbour interactions,

$$\frac{k_BT}{\tilde{\gamma}a} = \sqrt{2}\left[\frac{\left(e^{-\varepsilon_{NNN}/2k_BT} + e^{-(\varepsilon_{NN}+\varepsilon_{NNN})/k_BT}\right)\left(1+e^{-(\varepsilon_{NN}+\varepsilon_{NNN})/k_BT}\right)}{\left(1+e^{-\varepsilon_{NNN}/2k_BT}\right)\left(1-e^{-(\varepsilon_{NN}+\varepsilon_{NNN})/k_BT}\right)^2}\right]. \tag{10}$$

Eq. (10) is the main result of this work and in order to check the validity of our expression we first consider the case that we have a

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