Fluctuations of steps on crystal surfaces

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Abstract

Fluctuations of isolated and pairs of ascending steps of monoatomic height are studied in the framework of SOS models, using mainly Monte Carlo techniques. Below the roughening transition of the surface, the profiles of long steps show the same scaling features for terrace and surface diffusion. For a pair of short steps, their separation distance is found to grow as $t^{1/3}$ at late stages. Above roughening, simulational data on surface diffusion agree well with the classical continuum theory of Mullins.

Key words: Monte Carlo simulations, SOS model, terrace diffusion, step fluctuations, surface diffusion

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1. Introduction

In recent years, the dynamics of steps of monoatomic height on crystal surfaces has attracted much interest, both experimentally and theoretically. Experimentally, fluctuations of isolated steps as well as trains of steps on vicinal surfaces have been studied thoroughly [1].

Theoretically, three distinct mechanisms driving the step fluctuations have been identified, step diffusion, evaporation–condensation and terrace diffusion. Predictions of Langevin descriptions [2–5] have been checked, confirmed, and extended in Monte Carlo simulations on discrete SOS models [2,6,7]. Recently, extensive simulations on step diffusion and evaporation–condensation have been performed, for isolated and pairs of ascending steps [7]. Here, results of a related study on terrace diffusion will be presented.

Of course, the roughness of the surface crucially influences the step dynamics. Below the roughening transition temperature, $T < T_R$, the surface is smooth. Terrace diffusion may now be described in different ways. In an idealized description, the elementary move consists of the detachment of a step atom, followed by its random walk on the perfectly flat terrace, and the final attachment of the atom at the same or neighbouring step. This description may be simplified further by assuming that the time of the random walk may be neglected compared to that of the step processes. More realistically, terrace diffusion results from jumps of each surface atom to neighbouring sites. This type of kinetics is usually called surface dif-
fusion, and, in the following, only the idealized kind of kinetics will be called terrace diffusion. Obviously, step positions are uniquely defined for terrace, but not for surface diffusion. One of the aims of the present Monte Carlo study is to compare simulational data, in the framework of SOS models, for terrace diffusion and surface diffusion.

Above the roughening transition, steps are definitely no longer microscopically well defined; so the analysis will be restricted to surface diffusion. One may study the evolution of the profile of initially straight steps. Indeed, the corresponding equilibration problem, at $T > T_R$, has been described by Mullins many years ago [8], and we shall compare our Monte Carlo findings to that classical theory. Likewise, some of our findings at $T < T_R$ may be compared not only to Langevin theories on step fluctuations but also to theories on the equilibration of surface profiles [9–12].

The article is organized accordingly, presenting first our results on isolated and pairs of ascending steps below roughening, and then those on steps above roughening.

2. Below roughening

We simulate square surfaces with isolated and pairs of steps of monoatomic height. Initially, at time $t = 0$, the steps are perfectly straight, and the bordering terraces are perfectly flat; pairs of steps are usually separated by at most one lattice spacing. Step fluctuations result from terrace or surface diffusion.

In case of terrace diffusion, the acceptance rates of detaching and attaching atoms at steps, with a random walk in between, is assumed to be given by the Boltzmann factor of the change in the kink energies as described by the one–dimensional SOS model. There the kink energy is proportional to the number of missing bonds to the neighbouring step sites, i.e. $\epsilon |u^s(l) - u^s(l \pm 1)|$, $u^s(l)$ being the position of step $s$, ($s=1$, 2), at site $l$. The time unit, one Monte Carlo step (MCS), is assigned to $L$ (or $2L$) attempted elementary moves for isolated (pairs of) steps of length $L$. In case of pairs of steps no crossing of steps is allowed. To speed up simulations, one may replace the actual random walk by a probability distribution [3,6].

In case of surface diffusion, the acceptance rates for jumps of surface atoms to neighbouring sites will be given by the Boltzmann factor of the corresponding energy change of the two–dimensional SOS model, where the local energy is given by $\epsilon |h(i,j) - h(i',j')|$, with $(i,j)$ and $(i',j')$ being neighbouring surface sites. The roughening transition is known to occur at $k_BT_R/\epsilon \approx 1.25$. The time unit, one MCS, is assigned to $LM$ attempted jumps, where $L$ is the step length, say, $j = 1, \ldots, L$, and $M$ refers to the other direction of the surface. To monitor the step fluctuations, we recorded the step profile, $z(i,t) = \langle \sum h(i,j) \rangle / L$, summing over $j$ and averaging over $N$ Monte Carlo realizations with different random numbers. To stabilize the steps, the heights at the boundary lines parallel to the initial straight steps are kept constant during the simulation, e.g. for pairs of steps at $h=0$ and $h=2$.

The step dynamics may be described, both for surface and terrace diffusion, by the time evolution of the step profile $z(i,t)$, and, for terrace diffusion, by the average step positions, $u^s_0(t)$, and the fluctuation function $w^s(t) = \sqrt{\langle (u^s(t) - u^s_0(t))^2 \rangle}$, averaging over step sites and realizations.

Typical step profiles, for isolated and pairs of steps, are depicted in Fig. 1. To analyse their scaling behaviour, we use the ansatz $z(i,t) = z_f (i/t^{b_f})$. At a given height, $z = z_f$, one may yield at each time, by interpolation, the corresponding distance $i_f(t)$, and thence, setting $i_f \propto t^{b_f}$, one may obtain an effective exponent $b_f(t, z_f)$. Of course, full scaling holds only when $b_f$ eventually becomes independent of time $t$ and $z_f$.

Indeed, for rather long steps, of at least a few hundred sites, terrace diffusion and surface diffusion lead to consistent Monte Carlo results on the effective exponent $b_f$. Most of the simulations were done at $k_BT/\epsilon= 1.0$ and 0.8 for surface dif-
Fig. 1. Simulated step profiles $z(i, t)$ of the two-dimensional SOS model at $k_B T/\epsilon = 1.0$ with $44 \times 1000$ sites at $t = 0$ (circle), 6000 (square), 30000 (diamond), and 120000 (triangle) MCS, using surface diffusion. Averages have been taken over 70 realizations.

3. Above roughening

We studied isolated and pairs of ascending steps in the framework of two-dimensional SOS models at $T > T_R$, or one-dimensional SOS models, which are rough at all temperatures $T > 0$, computing the step profiles $z(i, t)$, applying surface diffusion. All cases lead to similar results, because above roughening individual steps are smeared out completely.

In particular, the step profiles scale, already
Fig. 2. Part of simulated step profile for isolated steps of monoatomic height above roughening. Data for the one-dimensional SOS model at $k_B T/\epsilon = 1.0$ with 152 sites have been taken at 1 (circle), 1000 (square) and 5000 (diamond) MCS, averaging over $10^6$ realizations.

at moderate times of typically a few $10^4$ MCS, with the critical exponent $b \approx 1/4$, the effective exponent $b_f$ depending only very weakly on $z_f$. The profiles show oscillations, with the amplitude decreasing rapidly with distance from the center of the surface, see Fig. 2. The onset of the oscillations may be readily understood by calculating the energetics of the first few excitations, starting from flat terraces and straight steps. Already the first move leads to an overshooting of the profile at the next-nearest distance from the center, $i = 0$, which again triggers an undershooting at further distance, and so on. This effect has been described before by Mullins in a continuum theory of surface equilibration above roughening [8]. Note that the oscillations persist to temperatures below roughening, as discussed above; however, the amplitudes become much smaller, at least at the times used in our Monte Carlo study, see also Fig. 1.

In Mullins’ theory, the basic equation reads $dz/dt = -A(d^4z/dx^4)$, where $A$ is a temperature dependent coefficient; the continuum variable $x$ corresponds to $i$ in the discrete description. The equation may easily be solved by Fourier analysis [8]. The resulting step profiles resemble closely those found in the simulations; differences are expected to show up only at early stages of equilibration, as observed before for other surface defects such as periodic grooves [13]. From the basic equation, it follows that the amplitudes of the oscillations settle at fixed values, independent of temperature. We confirmed these features by simulating steps at various temperatures. Actually, the continuum description of Mullins leads to a perfect scaling of the step profiles with $b = 1/4$.

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References

[1] H. C. Jeong and E. D. Williams, Surf. Sci. Rep. 34 (1999) 175.
[2] N. C. Bartelt, T. L. Einstein, and E. D. Williams, Surf. Sci. 312 (1994) 411.
[3] B. Blagojevic and P. M. Duxbury, in: Dynamics of Crystal Surfaces and Interfaces, Eds. P. M. Duxbury and T. Pence (Plenum, New York, 1997), p. 1; Phys Rev. E 60 (1999) 1279.
[4] S. V. Khare and T. L. Einstein, Phys Rev. B 57 (1998) 4782.
[5] A. Pimpinelli, J. Villain, D. E. Wolf, J. J. Metois, J. C. Heyraud, I. Elkinani, and G. Uimin, Surf. Sci. 295 (1993) 143.
[6] M. Bisani and W. Selke, Surf. Sci. 437 (1999) 137.
[7] F. Szalma, W. Selke, and S. Fischer, Physica A 294 (2001) 313.
[8] W. W. Mullins, in: Metal Surfaces: Structure, Energetics, and Kinetics, Eds. R. Vanselow and R. Howe (Springer, New York, 1963), p. 17.
[9] A. Rettori and J. Villain, J. Phys.–Paris 49 (1988) 257.
[10] H. Spohn, J. Phys. I 3 (1993) 69; J. Hager and H. Spohn, Surf. Sci. 324 (1995) 365.
[11] N. Israeli and D. Kandel, Phys. Rev. B 62 (2000) 13707; A. Chame and J. Villain, Phys. Rev. E 6302 (2001) 6104.
[12] H. P. Bonzel, Interface Sci. 9 (2001) 21.
[13] W. Selke and P. M. Duxbury, Z. Physik B 94 (1994) 311; Phys. Rev. B 52 (1995) 17468.