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Application of statistical tests to Monte Carlo simulations of crystal surface structures

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Abstract. Using the Monte Carlo technique we simulated single steps on Kossel-type crystal surfaces under equilibrium conditions up to the temperature region where statistical theories excluding overhanging step edge (ledge) configurations are questionable. We varied the ledge length between 40 and 960 units leading to average maximal step widths up to 40 units, so reaching dimensions observable with modern electron-optical techniques. We investigated jump and pair frequency distributions of the ledge after an equilibrium state was reached by direct tracing of its successive paths over the surface. The distributions were compared with those of an analytical low temperature step model. Hence the 'measured' distributions have to represent an average equilibrium distribution. The expected probability distributions are exponential and the sequence in the simulation introduces a dependence between successive samples. To be able to use statistical techniques in this case we developed criteria for the equilibrium distribution, the independence of successively sampled ledges and the minimal required ledge length.

1. Introduction

For the development of crystal growth theories knowledge of the structure of the crystal surface is very important. This is easy to see, because this structure determines the capability of the crystal to incorporate particles from the parent phase, i.e. the growth rate. For the sake of simplicity, in crystal growth theories the crystal is often assumed to be 'simple cubic' and composed of cubic blocks or units. These are identified with the atoms or molecules of the crystal. From a more general point of view, we may consider these units to correspond with the filled cells of an infinite three-dimensional lattice of cells. The boundary between the filled and empty cells, the interface, represents the surface of the crystal.

The state of the surface depends on the interactions between the (particles in the) cells and the temperature. Here we consider only nearest-neighbour interactions between filled cells. We use an interaction parameter ω, inversely proportional to the absolute temperature. At zero degrees Kelvin the surface is perfectly flat. At higher temperatures the surface becomes gradually rougher. Finally, at the critical temperature the surface ceases to exist, as both phases become identical.

On a real crystal surface steps may be present, for instance due to lattice imperfections. We speak of a monatomic step when two adjacent regions on the surface have a height difference of one atom. The possibilities to apply statistical tests to the structural properties of the boundary between simulated terraces, the step edge or ledge, are of prime interest in this paper. In figure 1 stepped surfaces are shown at increasing

temperatures and it can be seen that with increasing temperature: (i) the roughness of the surface and the ledge increases; and (ii) the number of overhanging ledge configurations (cf figure 2) increases. At low temperatures (figure 1(*a*)) the surface layer can be adequately described by a two-dimensional two-phase lattice cell system.

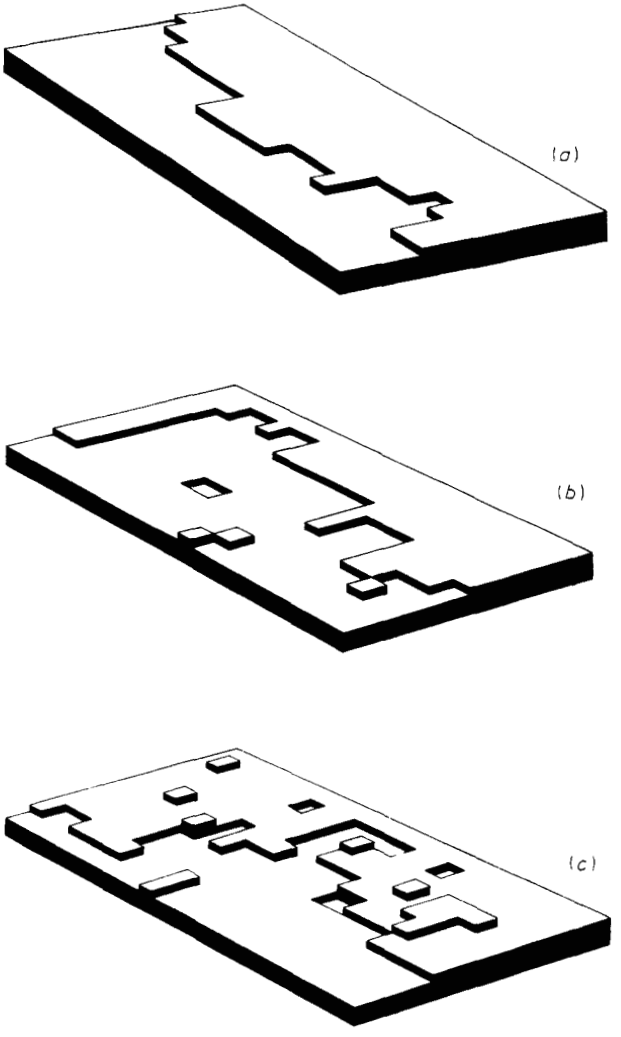

Figure 1. Computer drawn surfaces for: (*a*) $\omega = 1{\cdot}4$; (*b*) $\omega = 1{\cdot}2$; and (*c*) $\omega = 1{\cdot}0$, where $\omega \propto T^{-1}$ and T is the absolute temperature. The figures show that the surface and the ledge become rougher with increasing temperature. In (*c*) ledge overhangs can be seen.

Upon introducing the solid-on-solid constraint in the two-dimensional lattice system, the BCF step model (Burton *et al* 1951) results. In this model:

(i) one phase is completely filled;
(ii) the other phase is completely empty; and
(iii) ledge overhangs are not allowed.

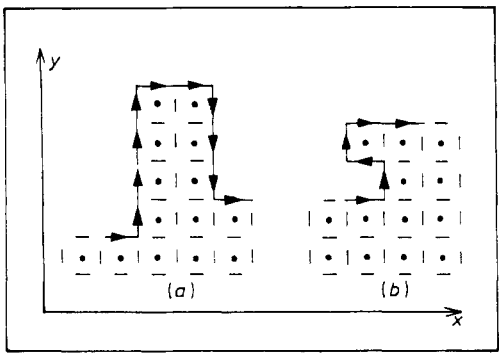

Figure 2. Top view on a surface in the two-dimensional simulation model (cf figure 1). The full line represents a ledge. One of the terraces is indicated by dots. (*a*) Part of a ledge with successive jumps of sizes 4, 0 and −3, contributing the pairs (., 4), (4, 0), (0, −3) and (−3, .) to the pair frequency distribution. (*b*) Part of a ledge with an overhang. Three successive jumps are shown with sizes 1, 1 and 0, respectively.

It can be seen in figure 1(*a*) that this model describes the low temperature situation rather well. The ledge in the BCF model is schematized in figure 3. Following the ledge along the x direction, jumps of various sizes can be seen in the y direction. According to BCF, the probability r_i of a jump of size i is given by:

$$r_i = \frac{1-\eta}{1+\eta}\eta^{|i|}, \tag{1}$$

where

$$\eta = \exp(-\omega). \tag{2}$$

Successive jumps in the ledge are not correlated. So

$$r_{ij} = r_i r_j, \tag{3}$$

where r_{ij} is the probability of finding a pair of adjacent jumps with sizes i and j, respectively.

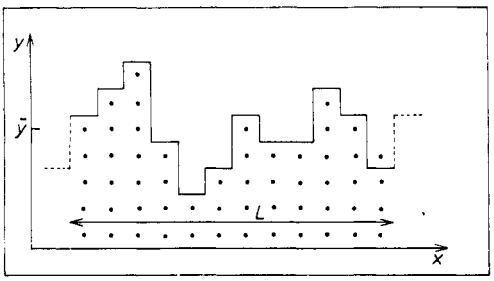

Figure 3. In the BCF step model part of the cells in the two-dimensional lattice are filled (indicated by dots in the figure). The step edge, parallel to the x axis, does not possess overhangs. Apart from the step length, the model is compatible with the one-dimensional simulation model; the figure shows a ledge of length $L = 12$ with periodic boundaries (indicated by the broken lines).

As will be explained in the next section, we are able to generate series of stepped surfaces with the Monte Carlo technique. Figures 1(*a*), (*b*) and (*c*) show parts of such surfaces at different temperatures. It can be seen that the neglect of ledge overhangs is not allowed at higher temperatures. In our temperature region ($1{\cdot}4 > \omega > 1{\cdot}0$) the density of ledge overhangs increases exponentially from the order of the density of jumps with size $i = 3$ to $i = 1$ (van Leeuwen and Mischgofsky 1975, cf also figure 6). Therefore the BCF formalism becomes questionable, particularly in the following aspects.

(i) Will the jump distribution still be described by equation (1)?

(ii) Will the high density of ledge overhangs introduce correlation between jumps?

In this paper we will investigate the possibility of applying the χ^2 test on data sampled by tracing successively simulated ledges to answer both questions. However, the expected jump distribution is exponential, and this causes the expected frequencies to be very low for high values of $|i|$. Further, due to the way we generate the stepped surfaces, it is necessary to check whether the 'measured' distributions really represent an average equilibrium distribution.

Two more difficulties are encountered in applying the χ^2 test to our data. Equations (1) and (3) hold for a step of infinite length on an infinitely large surface. Obviously, we are restricted to the simulation of relatively small surfaces. Finally, successively sampled distributions must be independent.

To overcome these problems, it was necessary in addition:

(i) to scrutinize in some cases the contributions of all individual terms to the value of χ^2;

(ii) to introduce two hypotheses concerning the equilibrium state of a ledge; and

(iii) to simulate the BCF step model as a reference.

We will return to the subject after a brief discussion of the simulation models.

2. The simulation models

2.1. Two-dimensional simulation model

With the Monte Carlo technique a stepped surface can be simulated: units are added to the surface (created) and removed from the surface (annihilated) at random positions, according to rules that ensure that the configurations generated this way follow Boltzmann statistics (Gilmer and Bennema 1972). The execution of a creation or annihilation depends on the number of bonds of the particle and a random number. In a simulation experiment n_c creations (and about the same number of annihilations) are executed.

The stepped surface is represented by a matrix; the elements give the position of the units at the surface relative to a reference plane. Periodic boundary conditions are applied to give units at the edges of the matrix four neighbours also. The ledge is chosen to be parallel to the longer side of the matrix (cf figure 1). In this simulation model ledge overhangs are allowed. The path of the ledge is determined n_s times per simulation experiment, i.e. at intervals of n_c/n_s creations. This yields the pair frequency distribution P_{ij} and the ledge overhang density h, defined as the average length of the ledge path in the reverse (i.e. $-x$) direction per unit step length (cf figure 2).

We repeated a simulation experiment for a certain value of ω several times. For the initial matrix of a new experiment we always took the final matrix of the preceding

experiment. The initial matrix of a new series of experiments generally does not have the right structure. After a transient period an equilibrium structure is obtained. This can be checked by the convergence of the data of surface properties, e.g. the surface energy. We only used data obtained after the equilibrium state was reached.

Successively generated matrices are very much alike: they differ in the occupancy of one cell at the most. If the number n_c of creations between two successive determinations of the ledge structure is small, the ledges are still very similar (only a fraction of all creations takes place at the ledge). This means that the observations used in applying the χ^2 test are not independent. Therefore, we have to make sure that a considerable difference between successively determined ledge structures exists: at each ledge position a large number of creations must have been executed. This can be achieved by choosing a high value for the number N of creations at the step per unit step length in each interval:

$$N = \xi n_c / L. \tag{4}$$

Moreover, the step length L and the total sample size $P \approx n_s L$ should be large enough. Since the computer time for an experiment is limited, we have to find minimum values for L and N for large enough values of P.

2.2. One-dimensional simulation model

In the one-dimensional simulation model (see figure 3) the ledge is represented by an array in which the elements give the position of the ledge. To obtain the pair frequency distribution the path of the ledge is now followed over its whole length. In this model ledge overhangs cannot occur.

It is easy to see that this model is more 'efficient' than the two-dimensional simulation model because all events take place at the ledge. So similar experiments require much less computer time. We will use this model to find the minimum values for N and L for which the hypotheses concerning the distributions are not rejected.

3. Hypotheses

We have at our disposal the observed pair frequency distribution P_{ij} of the number of adjacent jumps of sizes i and j. From this the jump frequency distribution P_i can be derived:

$$P_i = \tfrac{1}{2}(P_{i.} + P_{.i}) \tag{5}$$

with

$$P_{i.} = \sum_j P_{ij} \tag{6}$$

and

$$P_{.i} = \sum_j P_{ji}. \tag{7}$$

The periodic boundary conditions in the one-dimensional simulation model imply:

$$P_{i.} = P_{.i} \tag{8}$$

The total number P of jumps of any size is given by:

$$P = \sum_i P_i. \tag{9}$$

Now the estimates $\hat{p}_i$ and $\hat{p}_{ij}$ of the probabilities p_i and p_{ij} can be obtained from the frequency distributions P_i and P_{ij}

$$\hat{p}_i = P_i/P \tag{10}$$

$$\hat{p}_{ij} = P_{ij}/P. \tag{11}$$

In our simulations the average step direction is conserved by the periodic boundary conditions. In equilibrium, because of symmetry considerations, the observed distributions should not reject the following hypotheses:

$$H_1: \qquad p_i = p_{-i} \tag{12}$$

and

$$H_2: \qquad p_{ij} = p_{ji} = p_{-j,-i} = p_{-i,-j}. \tag{13}$$

To check whether the experimentally obtained jump frequency distribution is compatible with the theory mentioned above (cf equation (1)), the following hypothesis is tested:

$$H_3: \qquad p_i = r_i \tag{14}$$

with $r_i (i = \ldots, -1, 0, 1, \ldots)$ known constants, because ω is known. It is also interesting to investigate the occurrence of jump correlation in the two-dimensional simulation experiments (cf equation (3)). Therefore we test the hypothesis:

$$H_4: \qquad p_{ij} = p_i p_j. \tag{15}$$

The hypotheses mentioned above can be tested using the χ^2 test.

Testing the hypotheses H_1, H_2, H_3 and H_4 means testing the compatibility of a set of observed and expected frequencies. We will use the following theorem (Hoel 1962). *Theorem.* If $o_1, o_2, \ldots, o_m$ and $e_1, e_2, \ldots, e_m$ are the observed and expected frequencies, respectively, of the m possible outcomes of an experiment that is performed n times, then, as n becomes infinite, the distribution of the quantity

$$\sum_{i=1}^{m} (o_i - e_i)^2/e_i \tag{16}$$

will approach that of a χ^2 variable with ν degrees of freedom. ν is dependent on the hypotheses tested.

To test a hypothesis H_0 with a critical region 0·05 (we will use this value in the following), we evaluate the quantity χ^2 given by equation (16), taking care that all e_i comply with the hypothesis H_0, and with $\Sigma e_i = \Sigma o_i$. In the calculations we make sure that all expected frequencies exceed four. Then we determine the value of $\chi^2_{0\cdot95,\nu}$, which cuts off five per cent of the right tail of a χ^2 distribution with ν degrees of freedom. If $\chi^2 > \chi^2_{0\cdot95,\nu}$, the hypothesis is rejected at a level λ of over 95%, i.e. we state with a confidence of more than 95% that the hypothesis is not true. With every χ^2 goes a $\chi^2_{\lambda,\nu}$. We will present our results by giving values of the rejection levels $\lambda(H_i)$ rounded off upwards to the series of values 0·5–1–2·5–5–10–25–50–75–90–95–97·5–99–99·5 and 100%.

Of course the (decisive) power of the χ^2 test increases with increasing P. As mentioned before, the expected frequencies have to exceed four. The shape of the distributions involved makes it impossible to meet this requirement, however large we make P. Therefore we add up categories, as pointed out below.

For the hypotheses H_1 and H_3 the expected frequencies can be denoted by $\ldots, e_{-i}, e_{-i+1}, \ldots, e_0, \ldots, e_i, e_{i+1}, \ldots$. We now construct a new frequency distribution:

$$e'_{-k}, \ldots, e'_i, \ldots, e'_k$$

with

$$e'_{-k} = \sum_{i=-\infty}^{-k} e_i, \qquad e'_k = \sum_{i=k}^{\infty} e_i \tag{17}$$

and

$$e'_i = e_i \qquad \text{for } |i| < k,$$

where k is defined as the maximal value of $|i|$ for which all e'_i exceed four. For the hypotheses H_2 and H_4 the expected frequencies form two-way tables e_{ij} with $-\infty < i, j < \infty$. In an analogous way we construct a distribution e'_{ij} with $|i|, |j| \leqslant k$ and for example:

$$\begin{aligned} &e'_{ij} = e_{ij} \qquad \text{for } |i|, |j| \leqslant k, \\ &e'_{ik} = \sum_{j=k}^{\infty} e_{ij} \qquad \text{and} \qquad e'_{kk} = \sum_{i=k}^{\infty} \sum_{j=k}^{\infty} e_{ij}, \end{aligned} \tag{18}$$

where again k is defined as the maximal value of both $|i|$ and $|j|$ for which all e'_{ij} exceed four.

It is now possible to test the hypotheses H_1, H_2, H_3 and H_4. The specification of o'_i, e'_i and the number of degrees of freedom in terms of k are given in table 1.

Table 1. Table of observed frequencies o'_i and expected frequencies e'_i together with their number of degrees of freedom ν for the hypotheses H mentioned in the text.

H	o'_i	e'_i	ν
H_1	P'_i	$\frac{1}{2}(P'_i + P'_{-i})$	k
H_2	P'_{ij}	$\frac{1}{4}(P'_{ij} + P'_{ji} + P'_{-i,-j} + P'_{-j,-i})$	$3k^2 + 2k$
H_3	$\frac{1}{2}(P'_i + P'_{-i})$	Pr'_i	k
H_4	P'_{ij}	$P'_{i.}P'_{.j}/P$	$4k^2$

4. Results

4.1. The hypotheses of symmetry

4.1.1. One-dimensional simulation model. A number of 2500 exchanges per unit step length turned out to be sufficient to reach a steady state. Generally, we then used for each run values of $P > 48\,000$. This implies $k \geqslant 6$ for one-way tables and $k \geqslant 3$ for two-way tables.

As mentioned before, restrictions are laid upon the simulation and data sampling program with respect to the choice of N and L to obtain significant information. Moreover, in a well conducted experiment at least the hypotheses H_1 and H_2 have to be valid. Therefore we start testing these hypotheses for different values of N and L.

Table 2 shows a decreasing rejection level for increasing N at a constant value $L = 320$ for the length of the step. We conclude that for this step length $N = 0{\cdot}3$ is certainly too low, whereas $N = 6{\cdot}3$ is sufficient. From table 3 it follows for $N = 6{\cdot}3$ that $L = 160$ is somewhat short, but $L \geqslant 320$ is sufficient. Interpreting these tables, one should remember that H_1 and H_2 are hypotheses of symmetry. So rejection of H_1 and H_2 leads to the conclusion that symmetry is absent. However, it might also be concluded that the χ^2 test is applied to inappropriate data, e.g. because of the dependence of the distributions of successively sampled ledges. The fact that H_1 and H_2 are no longer rejected for high enough values of N and L indicates that the latter conclusion is preferable. So we conclude that the influence of N and L is sufficiently eliminated for $N > 6$ and $L > 300$.

Table 2. Some experiments with steps of lengths $L = 320$ for $\omega = 1{\cdot}0$. The values of the rejection levels indicate that the test samples are independent for $N \geqslant 6$.

N	0·3	6·3	31·3
$10^{-3} n_e/L$	1·25	1·25	25·0
n_c	100	2000	10 000
$\lambda(H_1)$ (%)	100	90	25
$\lambda(H_2)$ (%)	100	1	10
$10^{-3} P$	1280	64	256

Table 3. Some experiments with steps of various lengths for $\omega = 1{\cdot}4$, $n_e/L = 1250$ and $N = 6{\cdot}3$. It can be seen that a minimal step length is required to ascertain that the samples represent an average equilibrium distribution.

L	160	160	320	320	480
$10^{-3} n_c$	1	1	2	2	3
$\lambda(H_1)$ (%)	97·5	50	50	75	25
$\lambda(H_2)$ (%)	97·5	50	10	50	25
$10^{-3} P$	32	32	64	64	96

In table 4 we show the results of eight experiments for $\omega = 1{\cdot}0$ and $1{\cdot}4$ which fulfil these requirements. In all cases $\lambda(H_1)$ and $\lambda(H_2)$ remain below 90%, i.e. the hypotheses H_1 and H_2 are not rejected at the 0·95 level. Figure 4 gives an impression of successive step profiles for $\omega = 1{\cdot}0$ and $L = 320$ with $N = 6$. It shows changing sequences of jumps, whereas the general form of the ledge remains quite unchanged. Figure 5 gives an impression of the changes in shape of successive step profiles when $N = 250$.

4.1.2. Two-dimensional simulation model. A number of 4×10^5 creations at the surface turned out to be amply sufficient to reach a steady state. We always used values of $P \geqslant 4400$. This implies $k \geqslant 4$ for the one-way tables and $k \geqslant 2$ for the two-way tables.

Table 4. Results of the experiments for $\omega = 1{\cdot}0$ and $\omega = 1{\cdot}4$ from the one-dimensional simulation model with $L > 300$ and $N > 6$.

Model	One-dimensional							
ω	1·0					1·4		
L	320		480			320		480
N	6·3	31·3	12·5			6·3		6·3
$10^{-5}n_e$	4	80	6			4		6
Run order	1	2	1	2	3	1	2	1
k for H_1, H_3	8	9	8	8	9	6	6	6
k for H_2, H_4	4	4	4	4	4	3	3	3
$10^{-3}P$	64	256	48	48	48	64	64	96
$(P_0 - Pr_0)(Pr_0)^{-1} \times 100\%$	+0·4	−1·1	−0·9	−0·6	−1·2	−1·2	−1·1	−1·0
$\chi^2(H_1)$	12·4	5·3	8·8	12·8	4·8	5·0	7·1	2·4
$\chi^2(H_2)$	32·9	42·6	51·8	58·1	37·5	22·2	29·3	25·4
$\chi^2(H_3)$	6·1	29·9	27·1	6·3	12·6	32·3	22·4	16·3
$\chi^2(H_4)$	46·8	66·7	64·4	71·6	50·6	31·5	23·5	41·0
$\lambda(H_1)$ (%)	90	25	75	90	25	50	75	25
$\lambda(H_2)$ (%)	1	10	50	75	5	10	50	25
$\lambda(H_3)$ (%)	50	100	100	50	90	100	100	99
$\lambda(H_4)$ (%)	10	75	75	75	10	50	5	75

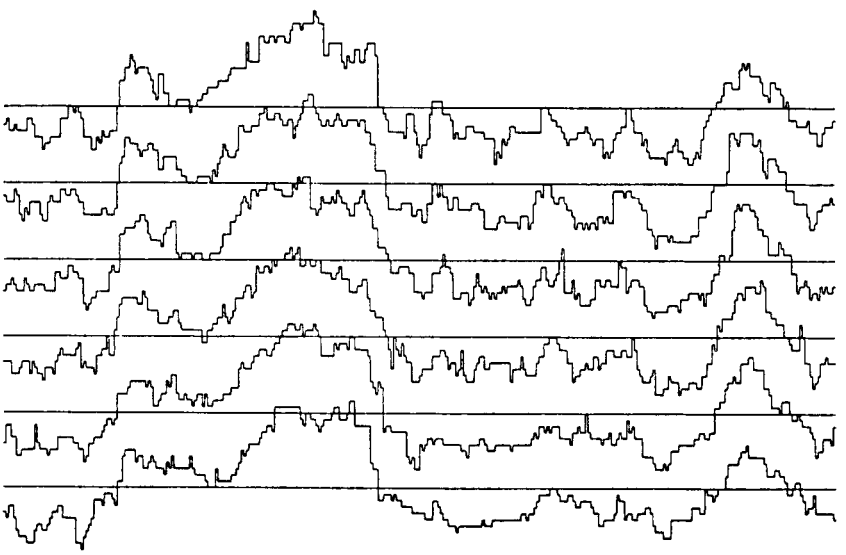

Figure 4. Successive patterns, obtained during an experiment for $\omega = 1{\cdot}0$, $L = 320$ and $N = 6$ in the one-dimensional simulation model. In order to see the jumps more clearly the vertical axis is expanded by a factor 2·5.

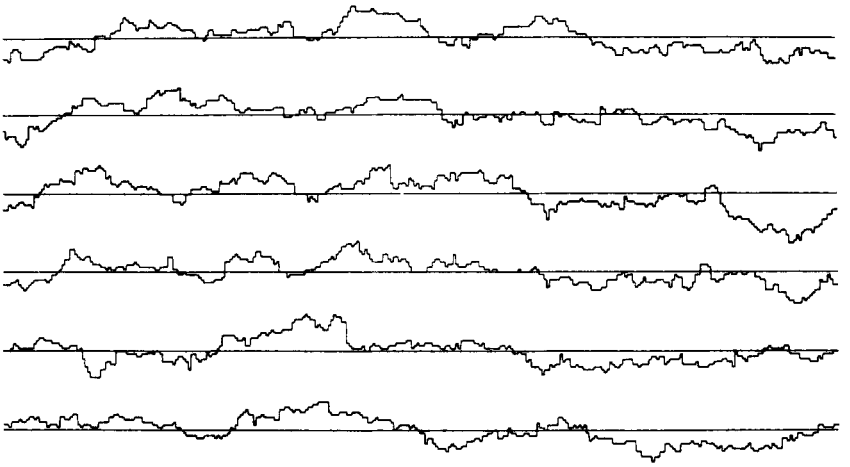

Figure 5. Time-dependent development of step profiles at intervals of 8×10^4 executed creations: $L = 320$, $\omega = 1{\cdot}0$ and $N = 250$.

To evaluate N it is necessary to estimate the fraction ξ of the total number of creations that takes place at the step. The estimated value of N exceeds six in all our experiments (see appendix). To keep computer time within reasonable limits, we took $L = 40$. Nevertheless, the values of the rejection levels $\lambda(H_1)$ and $\lambda(H_2)$ did not exceed 95%. So the hypotheses H_1 and H_2 are not rejected at a critical region of 0·05 (cf table 5).

Table 5. Results of the experiments for $\omega = 1{\cdot}0$ and 1·4 from the two-dimensional simulation model with $L = 40$ and $N \simeq 6$ (cf appendix).

Model	Two-dimensional			
ω	1·0		1·4	
L	40		40	
$n_c/L = N/\xi$	25		25	
$10^{-5} n_e$	4		1·5	
Run order	1	2	1	2
k for H_1, H_3	6	6	4	4
k for H_2, H_4	3	3	2	2
$10^{-3} P$	11·1	10·7	4·4	4·4
$(P_0 - Pr_0)(Pr_0)^{-1} \times 100\%$	−5·7	−2·6	−2·3	−2·8[a]
$\chi^2(H_1)$	10·3	5·7	2·6	5·9
$\chi^2(H_2)$	46·0	34·4	11·7	16·9
$\chi^2(H_3)$	62·3	63·0	9·7	6·4
$\chi^2(H_4)$	161	173	12·0	17·4
$\lambda(H_1)$ (%)	90	75	50	90
$\lambda(H_2)$ (%)	95	75	25	75
$\lambda(H_3)$ (%)	100	100	97·5	90
$\lambda(H_4)$ (%)	100	100	50	75

a The largest deviation here is $|(P_1 - Pr_1)/Pr_0| \times 100\% = 3{\cdot}1\%$.

4.2. Jump frequency distribution

4.2.1. One-dimensional simulation model. For $\omega = 1{\cdot}0$ hypothesis H_3 is rejected in two of the five experiments; for $\omega = 1{\cdot}4$ it is rejected in all three experiments (see table 4). So there is a strong indication that the hypothesis H_3 as a whole is not true. Inspection of P_i and Pr_i showed large absolute deviations of the expected frequencies for small jumps ($|i| = 0, 1$). Except in one case, always $P_0 < Pr_0$ and $P_1 > Pr_1$; the maximal absolute deviation always occurred for $i = 0$. However, in this case the relative deviation is rather small: $P_0 - Pr_0 < 0{\cdot}012\ Pr_0$ (see table 4). Moreover, for $|i| > 2$ the deviations between the expected and observed frequencies show to a reasonable extent a random pattern. Apparently, the hypothesis H_3 is rejected because of small systematic relative deviations between P_i and Pr_i for small values of i, and large but random relative deviations for higher values of i. Therefore it does not seem justified, in spite of the results of the test mentioned above, to reject the hypothesis H_3. This would be to favour alternative hypotheses, which are of no interest here. We conclude that $\hat{p}_i$ and r_i agree quite well: the absolute deviation never exceeds $0{\cdot}012 r_0$ (cf figure 6).

4.2.2. Two-dimensional simulation model. From the four experiments in table 5, H_3 was rejected only once for $\omega = 1{\cdot}4$ at the critical region 0·05. As ledge overhangs tend to split up large jumps into smaller ones, P_1 is much larger than Pr_1 for low values of ω.

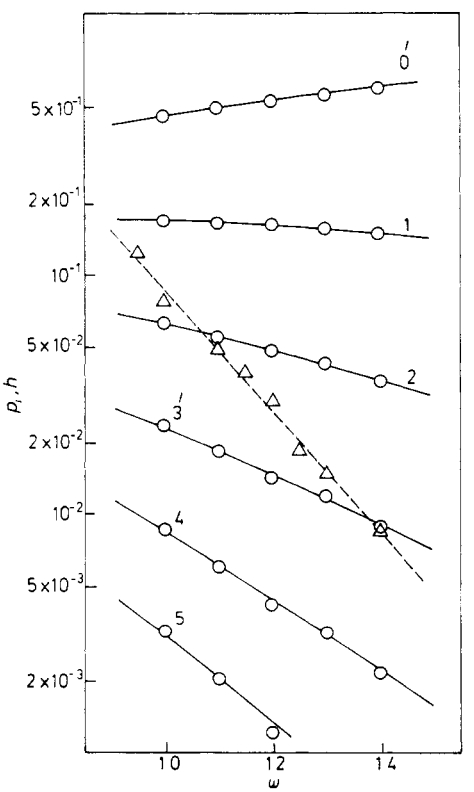

Figure 6. Jump density distribution and overhang density dependence on ω. ——— $r_i(\omega)$, BCF statistics (equation (1)); ○ $\hat{p}_i(\omega)$, one-dimensional model with $L = 320$; △ $h(\omega)$, two-dimensional model with $L = 40$; – – – – $h(\omega)$, best straight line (cf Burton *et al* 1951).

For example, for $\omega = 1{\cdot}0$ we find $(P_1 - Pr_1)/Pr_1 = 0{\cdot}03$. This results in a decrease of the other P_i, especially P_0 (see table 5 and figure 7). We can conclude that $\hat{p}_i$ and r_i agree within a maximal absolute deviation of about $0{\cdot}03r_0$ for $\omega = 1{\cdot}4$ and $0{\cdot}06r_0$ for $\omega = 1{\cdot}0$.

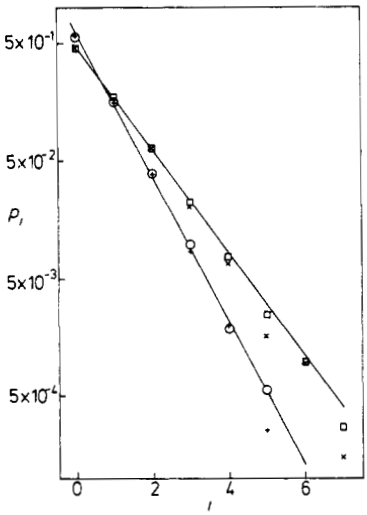

Figure 7. This plot of the jump density distribution for $\omega = 1{\cdot}0$ (□ and ×) and $\omega = 1{\cdot}4$ (○ and +) shows the influence of a short step length ($L = 40$) and overhangs on p_i. ——— r_i, BCF statistics (equation (1)); ○ and □ $\hat{p}_i$, one-dimensional model; + and × $\hat{p}_i$, two-dimensional model.

4.3. Jump correlation

4.3.1. One-dimensional simulation model. The rejection level for H_4 remains in all experiments below 75%, so H_4 is not rejected (see table 4). The contributions to χ^2 are randomly spread over all terms.

4.3.2. Two-dimensional simulation model. Table 5 shows that there is no jump correlation for $\omega = 1{\cdot}4$. For $\omega = 1{\cdot}0$, however, the hypothesis H_4 is rejected. We found that jump pairs (ij) with $|i| = |j| = 1$ strongly (about 50%) contributed to the value of χ^2.

Table 6. An example of the matrix A with $A_{ij} = (P'_{ij} - Pr'_i r'_j)/Pr'_j r'_j \times 100\%$ for $\omega = 1{\cdot}0$, $L = 40$ and $N \simeq 6$ (see appendix) in the two-dimensional simulation model. The cursive numbers clearly show the influence of overhangs on the correlation P_{ij} for sign i = sign j.

i \ j	−3	−2	−1	0	1	2	3
−3	*+0·1*	*+0·2*	*+0·1*	−0·0	−0·0	−0·1	+0·4
−2	*+0·8*	*+0·5*	*+0·2*	−0·0	−0·1	−0·3	0·0
−1	*+0·4*	*+0·4*	*+0·3*	−0·1	0·0	−0·1	−0·1
0	−0·2	−0·1	0·0	−0·1	0·0	−0·1	−0·1
1	−0·1	+0·1	−0·1	+0·1	*+0·5*	*+0·4*	*0·0*
2	−0·4	−0·4	0·0	−0·1	*+0·4*	*0·0*	*+0·1*
3	+0·1	−0·2	−0·2	−0·2	*+0·2*	*−0·1*	*−0·4*

It seems trivial to assume that the presence of jump correlation at higher temperatures is due to the ledge overhangs. For a given distribution of jumps, these increase the frequencies P_{ij} with sign i equal to sign j and decrease the frequencies P_{ij} with sign i not equal to sign j (cf figure 2). Indeed, this is strongly confirmed by our data.

Additional evidence for our assumption can be found in table 6, where we have given the relative deviation A_{ij} of P'_{ij} from Pr'_{ij}:

$$A_{ij} = (P'_{ij} - Pr'_{ij})/Pr'_{ij}. \tag{19}$$

Comparison of A_{11}, $A_{-1,-1}$ with $A_{1,-1}$, $A_{-1,1}$ shows the influence of ledge overhangs. The latter terms are not affected by these overhangs and almost follow the BCF law.

5. Conclusions

The structure of a step edge (ledge) on the surface of a Kossel crystal was studied, the surfaces being obtained by using the Monte Carlo simulation technique. Information about the structural properties of the ledge was obtained by following its path over the surface. At higher temperatures overhanging ledge configurations appeared, the overhang density h increasing from 0·008 at $\omega = 1{\cdot}4$ to 0·08 at $\omega = 1{\cdot}0$ (cf figure 6). To determine the influence of the overhang density on the jump density distribution and the pair density distribution we applied the χ^2 test.

To check the method, we also applied the test to a one-dimensional simulation model, because this model is correctly described by the theory. Using two hypotheses of symmetry we found that the test could be applied, provided: (i) the step is long enough ($L > 300$); and (ii) the number N of creations at the step between successive samples exceeds six. In spite of the rejection of hypothesis H_3: $p_i = r_i$, we found a reasonable correspondence between the simulation results and theory (cf figure 6). A short step length ($L = 40$) results in an increased number of short jumps and a decrease in the number of large jumps, relative to the values predicted by the theory for an infinite step (cf figure 7). In accordance with theory, the hypothesis of absence of jump correlation is not rejected.

In the two-dimensional simulation model we could only choose a rather short step length ($L = 40$), because of the computation times involved. Nevertheless, the hypotheses of symmetry were not rejected when the sample spacing (N) was large enough. In this model, the occurrence of large jumps is not only reduced by the short step length, but also by the presence of overhangs (cf figure 7). We concluded that generally $p_i = r_i$ within a maximal absolute deviation of 0·03 r_0 for $\omega = 1{\cdot}4$ and 0·06 r_0 for $\omega = 1{\cdot}0$. For $\omega = 1{\cdot}4$ hypothesis H_4 is not rejected, i.e. there is no jump correlation. For $\omega = 1{\cdot}0$, however, H_4 is rejected. We found that terms derived from jump pairs (i,j) with sign i = sign j (especially for $i, j = \pm 1$) contribute most to the value of χ^2, i.e. jump correlation in the two-dimensional simulation model results purely from the existence of overhangs.

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Appendix. Calculation of N in the two-dimensional simulation model

In the foregoing it appeared necessary to determine the number of executed creations at the step during the interval between two measurements of the ledge properties. In the two-dimensional simulation model only the number of executed creations on the surface is known. Therefore we must estimate the fraction ξ of all executed creations that take place at the ledge. We approximate ξ by the ratio of the creation flow to a ledge and the sum of the creation flows to a stepless surface and a ledge. The creation flows are given in equations (4) and (23) of Gilmer and Bennema (1972). A numerical value for the creation flow to a stepless surface can be obtained from the concentration of surface sites which can be created (given in table 2 of the same paper) and the kinetical coefficients (equations (2) and (3) of van Leeuwen and Mischgofsky 1975). The creation flow to a ledge can be estimated by assuming the concentration of kink sites to be 20%. For $\omega = 1{\cdot}0$ we find $\xi \approx 0{\cdot}16$ for a step of length $L = 40$ on a 20×40 surface. Taking a test sample of such a ledge every 1000 creations implies $N = 25\xi \simeq 4$. Because of the fact that for $\omega = 1{\cdot}0$ about 30% of the samples are omitted during a run, we can estimate that $N \simeq 6$. This also holds for $\omega = 1{\cdot}4$ as the creation flow towards the stepless surface decreases strongly with increasing value of ω.

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