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Simple formula for Miller indices of periodically kinked and stepped fcc surfaces

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A periodically kinked and stepped surface can be characterized by two integers for each step and two more integers to translate one step to its neighbor. In terms of these four integers, we write a simple formula for the Miller indices for fcc surfaces vicinal to {100} and to {111} planes. These useful formulas are extensions of the work of Van Hove and Somorjai [Surf. Sci. 92 (1980) 489].

With the recent growth of interest in stepped and kinked surfaces, there is considerable interest in characterizing these surfaces. Van Hove and Somorjai [1], hereafter VHS, introduced and systematized widely accepted nomenclatures for such surfaces and showed how, from the Miller indices, one can deduce the configuration of the surface. For many purposes, particularly when constructing model surfaces to use in computing energetics [2], one wants to proceed in the reverse direction and find the Miller indices for a specified surface. Thus, our goal was to write down a simple formula for the Miller indices in terms of readily obtainable lengths characterizing a periodically stepped and kinked surface. Our results are fully consistent with and perhaps implicit in VHS; they might best be viewed as modest corollaries or extensions. Nonetheless, we believe it will be helpful to have explicit rather than implicit formulas. In this short paper we focus on surfaces vicinal to the high-symmetry {100} and {111} faces of fcc crystals. Our approach could readily be generalized to other crystal structures and faces.

Because of its higher symmetry, the (100) face is somewhat easier to treat. Our nomenclature is illustrated in fig. 1. In general we describe the periodically kinked terrace edge by two integers, m_1 and m_2, which multiply $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$, respectively, two primitive vectors along the two principal directions of the close-packed step edges and with magnitude equalling the nearest-neighbor spacing. Both vectors have their origins at the "inner elbow" of the kink, i.e., at the site along the edge with the highest coordination. The vector $\boldsymbol{b}_1$ is directed along a $(11\bar{1})$ microfacet step edge: it is perpendicular to both (100) and $(11\bar{1})$ and so is parallel to vector [011]. Similarly, $\boldsymbol{b}_2$ is

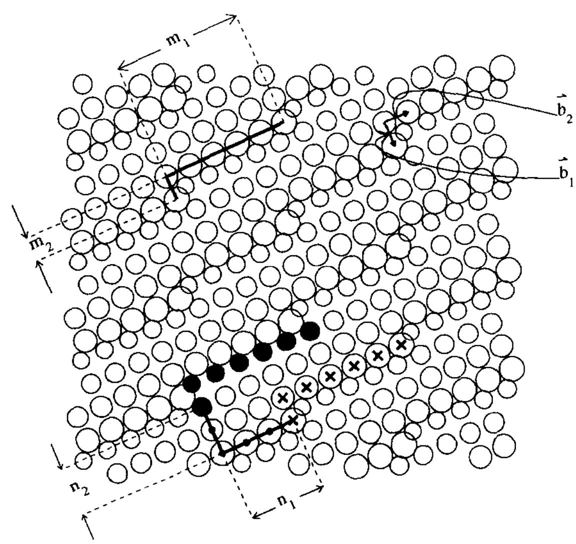

Fig. 1. Nomenclature for surfaces vicinal to (100), in this example $(163\bar{2})$. Here $m_1 = 5$, $m_2 = 1$, $n_1 = 3$, $n_2 = 2$.

directed along a (111) microfacet step edge and is parallel to $[01\bar{1}]$. The integers m_1 and m_2 represent the lengths of the $(11\bar{1})$ microfacet step edges and (111) microfacet step edges, respectively (in units of nearest neighbor distance). Then the vector $m_1\boldsymbol{b}_1 - m_2\boldsymbol{b}_2$, called $\boldsymbol{e}$ in VHS, connects neighboring kink "elbows" (or tips or any other common feature) on the same terrace edge.

We generally assume either m_1 or m_2 is at most one, so that we have simple kinks or straight steps. (If both were taken to be large, the resulting Miller index surface would probably partially fill in the large zig-zag of the terrace edge.) We next must characterize the two-dimensional translation vector that would carry one terrace into the next. If we start from an atom in a lower terrace just beyond the tip of a kink in the adjoining upper terrace, then the vector is $n_1\boldsymbol{b}_1 + n_2\boldsymbol{b}_2$, where n_1 and n_2 are integers. Less ambiguously, one can restate this idea by noting that comparable points on neighboring terraces are connected by a vector, called $\boldsymbol{w}$ in VHS, the projection of which in the (100) plane is $\boldsymbol{w}_{\rm p} = (n_1 + \frac{1}{2})\boldsymbol{b}_1 + (n_2 + \frac{1}{2})\boldsymbol{b}_2$. Assuming m_1 and m_2 have no common factors, the Miller indices for such surfaces are:

$$(h, k, l) = (2MN + m_1 + m_2,\ m_1 + m_2,\ m_2 - m_1), \quad (1)$$

where $MN \equiv m_1 n_2 + m_2 n_1$. A derivation is sketched in the appendix. If m_1 and m_2 are both odd, then h, k, and l are all even and should be divided by 2.

There are a number of checks and observations we can make about this expression. First, $\boldsymbol{w}_{\rm p}$ is not uniquely defined: the replacements

$$n_2 \to n_2 + jm_2,\ n_1 \to n_1 - jm_1 \quad (\text{for any integer } j) \quad (2)$$

lead to another such translation vector. This comment follows immediately from the observation that the Miller indices depend on n_1 and n_2 only through the product $MN \equiv m_1 n_2 + m_2 n_1$. Second, in this case only h in eq. (1) depends on $\boldsymbol{w}_{\rm p}$ or MN. Third, by exchanging indices 1 and 2, one should generate essentially the same substrate. Specifically, we see that h and k are unchanged while l reverses sign. The new surface is the original reflected through a (001) mirror plane. Fourth, we have constructed the Miller indices so that $h \geq k \geq l$. By using the lattice symmetries, here permutations, inversions, and reflections through principal directions, one can produce other sets of indices that correspond to physically identical substrates.

For straight steps, with edges in $\langle 011 \rangle$ directions, either m_1 or m_2 vanish, and we get simply

$$(h, k, l) = [m(2n+1),\ m,\ \pm m] \to (2n+1,\ 1,\ \pm 1). \quad (3)$$

This result, as well as the others for *unkinked* steps mentioned below, are listed concisely in table 1 of VHS. For steps with simple kinks, either m_1 or m_2 is 1; supposing $m_2 = 1$ gives

$$(h, k, l) = [m_1(2n_2 + 1) + 2n_1 + 1,\ m_1 + 1,\ 1 - m_1],\quad \{100\}, \quad (4)$$

which reduces to eq. (3) in the limit $m_1 \to \infty$. Eq. (4) can be inverted to yield

$$m_1 = (k - l)/(k + l) \quad (\text{for } m_2 = 1). \quad (5a)$$

(The quotient expression eliminates concerns about a common factor being removed from the indices.) With similar manipulating we can obtain $m_1 n_2 + n_1 = (h - k)/(k + l)$. As emphasized in conjunction with eq. (2), n_1 and n_2 are not uniquely defined by the simply-periodic vicinal surface, so that an inversion formula can only be expected to produce n's which are in the same family (via eq. (2)) as the originals. From eq. (2) we note that since $m_2 = 1$, every integer n_2 is in this family. For any n_2, the corresponding n_1 is

$$n_1 = \frac{h-k}{k+l} - n_2 \frac{k-l}{k+l} \quad (\text{for any integer } n_2). \quad (5b)$$

By direct substitution, it is easy to see that eqs. (5a) and (5b) satisfy eq. (4). Changing the value of n_2 corresponds to changing the indexing parameter j in eq. (2).

The case of jagged step edges, in the $\langle 001 \rangle$ directions, with $m_1 = m_2 = 1$, is just a special case of eq. (4):

$$(h, k, l) = [2(n_1 + n_2 + 1),\ 2,\ 0] \to (n_1 + n_2 + 1,\ 1,\ 0). \quad (6)$$

The (111) surface has only 3-fold, not 6-fold symmetry. As illustrated in fig. 2, we take $\hat{b}_1$ and $\hat{b}_2$ along $[01\bar{1}]$ and $[1\bar{1}0]$, so that they are on the edges of (100) and $(11\bar{1})$ microfacets, respectively. These steps have been called ⟨110⟩/{100} and ⟨110⟩/{111} [3], indicating their direction and microfacet orientation, or simply A and B, respectively [4]. Again, note that b_1 and b_2 are directed from an atom which has highest coordination to one of the neighboring atoms with lowest coordination. (Also, m_1 now describes the length of the (100) microfacet steps, and m_2 describes the length of the $(11\bar{1})$ microfacet steps.) Hence, $e = m_1 b_1 - m_2 b_2$ again connects neighboring kink "elbows" (or tips) on the same terrace edge. Starting once more from an atom in a lower terrace just beyond the tip of a kink in the adjoining upper terrace, the vector to a kink apex on the neighboring edge on the lower terrace is $n_1 b_1 + n_2 b_2$, where n_1 and n_2 are integers. Less ambiguously, again, comparable points on neighboring terraces are connected by a vector with component $w_p = (n_1 + \frac{1}{3})b_1 + (n_2 - \frac{2}{3})b_2$ in the (111) plane. In the appendix we show, with the same caveat as for eq. (1), that the Miller indices for such a surface are

$$(h, k, l) = (MN + 2m_1 + m_2,\ MN + m_2,\ MN - m_2),$$
$$MN \equiv m_1 n_2 + m_2 n_1. \qquad (7)$$

Of course, as before, if all three indices are even, we must divide by 2.

In this case we see that all indices depend on the translation vector between terraces. Again, the replacements of eq. (1) leave the indices invariant, as must be true on physical grounds. Now, however, there is no symmetry involving interchange of subscripts 1 and 2. We also note that $(k-l)/2 = m_2$ and $(h-k)/2 = m_1$. Since the steps have unit height, these numbers are just the number of $(11\bar{1})$ and (100) microfacet unit cells, as in eq. (18) of VHS. The number of (111) unit cells is $m_1 n_2 + m_2 n_1 = k + l$, again agreeing with VHS. Again we have constructed the Miller indices so that $h \geq k \geq l$. A straight A or (100) step has $m_2 = 0$; hence,

$$(h, k, l) = [m_2(n_2+2),\ m_1 n_2,\ m_1 n_2] \rightarrow (n_2+2,\ n_2,\ n_2). \qquad (8)$$

A straight B or $(11\bar{1})$ step has $m_1 = 0$; hence,

$$(h, k, l) = [m_2(n_1+1),\ m_2(n_1+1),\ m_2(n_1-1)] \rightarrow (n_1+1,\ n_1+1,\ n_2-1). \qquad (9)$$

A kinked A or (100) step has $m_2 = 1$; hence,

$$(h, k, l) = [m_1(n_2+2) + n_1 + 1,\ m_1 n_2 + n_1 + 1,\ m_1 n_2 + n_1 - 1]. \quad \{\mathbf{111}\}\mathrm{A}. \qquad (10)$$

Inverting, we find

$$m_1 = (h-k)/(k-l) \quad (\text{for } m_2 = 1) \qquad (11a)$$

and, thence, $m_1 n_2 + n_1 = (k+l)/(k-l)$. From eq. (7) we see that, as in eq. (4), the n's only enter the Miller indices via the product MN. With the same reasoning accompanying eq. (5b), we now find

$$n_1 = \frac{k+l}{k-l} - n_2 \frac{h-k}{k-l} \quad (\text{for any integer } n_2). \qquad (11b)$$

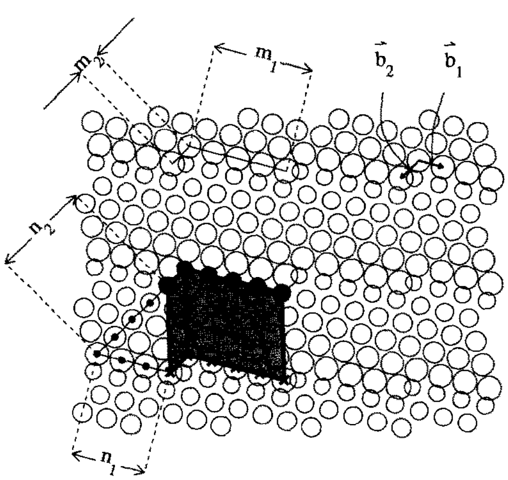

Fig. 2. Nomenclature for surfaces vicinal to (111), in this example (14109). Here $m_1 = 4$, $m_2 = 1$, $n_1 = 3$, $n_2 = 4$. The bold lines outline the shaded (111) microfacet of a (14109) unit cell, in this example containing 19 unit cells, as discussed in the appendix.

A kinked B or $(11\bar{1})$ step has $m_1 = 1$; hence,

$$(h, k, l) = [n_2 + m_2(n_1+1) + 2, \quad n_2 + m_2(n_1+1),\ n_2 + m_2(n_1-1)]. \quad \{111\}\text{B}. \tag{12}$$

Inverting gives

$$m_2 = (k-l)/(h-k) \quad (\text{for } m_1 = 1) \tag{13a}$$

and $m_2 n_1 + n_2 = (k+l)/(h-k)$. It is now n_1 that can take on all integer values, so that

$$n_2 = \frac{k+l}{h-k} - n_1 \frac{k-l}{h-k} \quad (\text{for any integer } n_1). \tag{13b}$$

For jagged step edges, $m_1 = m_2 = 1$, and

$$(h, k, l) = (N+3,\ N+1,\ N-1), \quad N \equiv n_1 + n_2. \tag{14}$$

Similar results could be obtained for bcc crystals. In that case, of course, the close-packed face is (110) rather than (111); since the stacking is ABAB rather than ABCABC, there is just one kind of step with close-packed spacing along the edge.

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Appendix: Outline of derivation

A surface with Miller indices (hkl) can be decomposed into three types of microfacets, two if the edges are unkinked. If $h \geq k \geq l$, the decomposition is:

$$(hkl) = \tfrac{1}{2}(k+l)(111) + \tfrac{1}{2}(k-l)(11\bar{1}) + (h-k)(100). \tag{A.1}$$

Following VHS, one can find the ratios of the areas of each microfacet in terms of the number of unit cells in each microfacet. If

$$(hkl) = a(111) + b(11\bar{1}) + c(100) \tag{A.2}$$

then, using VHS notation for microfacet surface area ratios:

$$n_{[hkl]} : n_{[111]} : n_{[11\bar{1}]} : n_{[100]} = \begin{cases} 2:4a:4b:2c & \text{if } hkl \text{ not all odd,} \\ 4:4a:4b:2c & \text{if } hkl \text{ are all odd.} \end{cases} \tag{A.3}$$

For example,

$$(14\,10\,9) = \tfrac{19}{2}(111) + \tfrac{1}{2}(11\bar{1}) + 4(100),$$

$$n_{[14\,10\,9]} : n_{[111]} : n_{[11\bar{1}]} : n_{[100]} = 2:38:2:8 = 1:19:1:4.$$

That is, in each $(14\,10\,9)$ unit cell there are 19 (111) unit cells, a $(11\bar{1})$ unit cell, and four (100) unit cells.

Consider steps vicinal to (111). Since the steps are of monatomic height, $n_{[11\bar{1}]} : n_{[100]}$ gives the ratio of the length of the $(11\bar{1})$ microfacet edge (or B edge) to the length of the (100) microfacet edge (or A edge). In the above example (cf. fig. 2) of a $(14\,10\,9)$ surface, $n_{[11\bar{1}]} : n_{[100]} = 1:4 = m_2 : m_1$. Next, $n_{[111]}$, the number of (111) unit cells, is given by $m_2 n_1 + m_1 n_2$, here 19. In summary,

$$n_{[111]} : n_{[11\bar{1}]} : n_{[100]} = m_2 n_1 + m_1 n_2 : m_2 : m_1. \tag{A.4}$$

Using eq. (A3):

$$m_2 n_1 + m_1 n_2 : m_2 : m_1 = 4a:4b:2c = a:b:c/2 \tag{A.5}$$

and hence

$$a = m_2 n_1 + m_1 n_2, \quad b = m_2, \quad c = 2m_1. \tag{A.6}$$

When inserted into eq. (A.2), eq. (A.6) leads directly to eq. (7).

Similarly, eq. (1) can be derived for surfaces vicinal to (100). In this case,

$$n_{[111]} : n_{[11\bar{1}]} : n_{[100]} = m_2 : m_1 : m_1 n_2 + m_2 n_1 = a:b:c/2, \tag{A.7}$$

so that one inserts into eq. (A2) the values

$$a = m_2, \quad b = m_1, \quad c = 2(m_1 n_2 + m_2 n_1). \tag{A.8}$$

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