Lawrence Berkeley National Laboratory

Recent Work

Title

A NEW MICROFACET NOTATION FOR HIGH-MILLER-INDEX SURFACES OF CUBIC MATERIALS WITH TERRACE, STEP AND KINK STRUCTURES

Permalink

<https://escholarship.org/uc/item/3gq9p64s>

Author

Van Hove, M.A.

Publication Date

1979-07-01

Lawrence Berkeley Laboratory

UNIVERSITY OF CALIFORNIA, BERKELEY, CA

Materials & Molecular Research Division

Submitted to Surface Science

A NEW MICROFACET NOTATION FOR HIGH-MILLER-INDEX
SURFACES OF CUBIC MATERIALS WITH TERRACE, STEP AND
KINK STRUCTURES

M. A. Van Hove and G. A. Somorjai

July 1979

RECEIVED
LAWRENCE
BERKELEY LABORATORY

AUG 28 1979

LIBRARY AND
DOCUMENTS SECTION

TWO-WEEK LOAN COPY

*This is a Library Circulating Copy
which may be borrowed for two weeks.
For a personal retention copy, call
Tech. Info. Division, Ext. 6782*

LBL-9363 c. 2

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

A NEW MICROFACET NOTATION FOR HIGH-MILLER-INDEX SURFACES
OF CUBIC MATERIALS WITH TERRACE, STEP AND KINK STRUCTURES

M.A. Van Hove and G.A. Somorjai

Materials and Molecular Research Division, Lawrence Berkeley
Laboratory, and Department of Chemistry, University of
California, Berkeley, California 94720

Abstract

The ideal (i.e. unreconstructed and unrelaxed) structure of arbitrary high Miller index surfaces of cubic crystals is analyzed in terms of terraces, steps and kinks, and a new, simple and useful microfacet notation is proposed. The cubic crystals include the simple cubic, face-centered cubic, body-centered cubic, diamond, zincblende, NaCl and CsCl crystals.

1. Introduction Low energy electron diffraction (LEED) studies revealed

that unreconstructed, high Miller index crystal faces have atomic structures that exhibit ordered periodic steps of atomic height that separate terraces of atoms. The steps often have ledges or kinks as well.

With the exception of a few low Miller index surfaces it is difficult to visualize the atomic surface structure of various crystal surfaces when only their Miller indices are given. Inversely, it is difficult to determine the Miller indices of a surface from its terrace/step/kink structure or from its reciprocal lattice (LEED pattern). The interrelation of the atomic surface structure and the Miller index notation arises frequently during experimental studies of high Miller index surfaces. The unique structures of many of these surfaces strongly influence the chemical activity that is of great importance in heterogeneous catalysis and in forming surface chemical bonds.

The purpose of this paper is to investigate the structure of ideal high Miller index surfaces and to propose a nomenclature that permits the deduction of the atomic surface structure and easy correlations with other existing notations. Nicholas and coworkers⁽¹⁾ have developed a method of obtaining very useful partial information about ideal (i.e. unreconstructed, unfacetted, clean) surfaces with arbitrary (hkl) Miller indices: this information is the number of surface atoms with a given coordination number, i.e. with a given number of unbroken bonds. And Nicholas' atlas⁽²⁾ of surfaces with not-too-high Miller indices has provided a valuable source of information for many surface scientists to identify the structure of a variety of surfaces.

A step notation was introduced by Lang, Joyner and Somorjai⁽³⁾ for stepped and kinked surfaces, which has helped considerably in visualizing their structure. This step notation has the general form $n(h_t k_t l_t) \times (h_s k_s l_s)$, where

$(h_t k_t l_t)$ represents the terrace, $(h_s k_s l_s)$ represents the step face and n measures the width of the terrace in number of atoms.

The step notation is exemplified by the fcc (775) surface for which the designation $6(111) \times (11\bar{1})$ shows that 6-atom-wide (111) terraces are separated by single-height (111) steps. Likewise the fcc(10,8,7) surface is denoted $7(111) \times (310)$, showing that the step itself is a (310) plane, i.e. a kinked step.

A stepped surface is usually defined as one with terraces of low Miller indices [such as (111), (100) or (110) for face-centered cubic (fcc) lattices], with constant widths and mono-atomic-height step faces which are also characterized by low Miller indices. Kinked surfaces have step faces that are themselves higher-index planes, i.e. are not planar but stepped. Each low Miller index piece of a surface we shall call a "microfacet", whether it is a terrace or a step face or a low Miller index component of a kinked step. The underlying idea of our analysis is that Miller indices can be decomposed as any normal vector in terms of simple vectors that represent low Miller index microfacets. For example, from the vector decomposition $(775) = 5(111) + 1(11\bar{1})$ one can directly learn that (111) terraces and simple steps of $(11\bar{1})$ orientation are present on the (755) crystal surface; the coefficients 5 and 2 can be interpreted, with rules to be described later, as the relative sizes of the terraces and the steps. This vector decomposition will also provide our new microfacet nomenclature.

We shall start out in Section 2 in two dimensions to explore in simple cases some of the characteristics of high Miller index surfaces. This will enable us to introduce our new microfacet notation in Section 3. We shall then generalize our considerations to three dimensions in Sections 4 and 5, concentrating on cubic materials with one atom per unit cell. In Section 6 we shall discuss other cubic

space lattices, and in Section 7 surfaces are classified into groups with common characteristics. The inverse problem, that of finding the Miller indices from structural information about the surface will be discussed in Section 8, where a table of surface structures that are identified by both the microfacet and Miller index notation is included for many surfaces

2. Examples of One-dimensional Surfaces of Two-dimensional Crystals

Figure 1 shows a variety of terminations of two-dimensional square crystals (these are the analogues in two dimensions of two-dimensional surfaces of three-dimensional crystals). The surfaces are designated by pairs of Miller indices (h,k) , using the same conventions as in three dimensions. In Figure 1a a $(1,2)$ surface is seen to be composed either of a $(1,1)$ microfacet (the step) and a $(0,1)$ microfacet (the terrace), or if one prefers, of one $(1,0)$ microfacet and a $(0,1)$ microfacet containing two unit cells of a $(0,1)$ surface. There is a certain arbitrariness in the choice of microfacets used for the decomposition; here, either the microfacets $(1,0)$ and $(0,1)$ or the microfacets $(1,1)$ and $(0,1)$ may be chosen.

In the following Sections we shall therefore analyze the decompositions without assuming any particular choice of microfacets, since different choices may be preferable in different cases.

The vector $(1,2)$ which is perpendicular to the $(1,2)$ surface, can be vectorially decomposed as $(1,2)=(1,1)+(0,1)$ or as $(1,2)=(1,0)+2(0,1)$; thus, a vectorial decomposition produces the microfacet structure described above in terms of vectors with simple coefficients, indicating also the correct relative size of the microfacets. In general, for this type of lattice the following simple decompositions can be performed:

$$(h,k) = h(1,0) + k(0,1)$$

or

$$(h,k) = \begin{cases} h(1,1) + (k-h)(0,1) & \text{if } h \leq k \\ k(1,1) + (h-k)(1,0) & \text{if } h \geq k. \end{cases}$$

These equations are already examples of our new microfacet notation, which will be slightly extended to provide more information.

In Figure 1b a (2,5) surface is seen to decompose into identical units consisting of one short terrace followed by one long terrace, with two steps in the unit. This is an example of a class of surfaces not usually considered, that of high Miller index surfaces that serve as "terraces" for even higher Miller index surfaces; here, a high Miller index (1,2) terrace has steps (an additional (0,1) unit cell at the edge of every other (0,1) microfacet), as one sees from $(2,5) = 2(1,2) + (0,1)$. We shall not analyze the structure of these "stepped stepped surfaces" in detail, but we point out that if none of the indices h, k is 1, the surface has this type of higher complexity. The complication is introduced as a result of requiring the presence of only mono-atomic height steps. As shown in Figure 1c one could obtain a simple (2,5) oriented surface with constant terrace width if we allowed multiple-height steps. However, we shall not consider multiple-height steps since single-height steps seem to predominate on stable high Miller index surfaces of fcc metals.

Since we shall have to deal with both face-centered and body-centered lattices in three dimensions, it is useful to consider at this point the effect of adding centered atoms to our two-dimensional crystals. Figure 1d shows how the vector decomposition $(1,2) = (1,0) + 2(0,1)$ is no longer meaningful in this case, while the notation $(1,2) = (1,1) + (0,1)$ is still useful. This is because no useful (1,0) microfacets occur in this case, while the (1,1) microfacet has become by far the more natural (close-packed) microfacet to consider. Thus, with different

types of lattices, different choices of microfacets will be more appropriate. Another observation is important as well: the (1,1) microfacet now has double the number of atoms as before and so the term (1,1) in the decomposition should now be interpreted to mean that two unit cells of the (1,1) microfacet are present in this case. Therefore, the prefactors of the vector decomposition acquire a different meaning: as far as counting unit cells on the microfacets is concerned, the prefactors should be weighted 2:1 when comparing (1,1) and (0,1) microfacets. Similar weights will apply on the surfaces of three-dimensional crystals. To include the numbers of unit cells of each microfacet in our notation, we shall insert them as subscripts in the decomposition, e.g.

$$(1,2) = 1_2(1,1) + 1_1(0,1).$$

3. A New Nomenclature for Arbitrary Surfaces of Cubic Materials

We propose here a new microfacet notation for high Miller index surfaces that is quite general, easy to use and informative. The general form will be

$$M(S) = [a_{n_1}^1 \text{uc}(h_1 k_1 \ell_1) + a_{n_2}^2 \text{uc}(h_2 k_2 \ell_2) + a_{n_3}^3 \text{uc}(h_3 k_3 \ell_3)] \quad (1)$$

where M is the chemical element,

S denotes a stepped (or kinked) surface;

$(h_i k_i \ell_i)$, $i = 1, 2, 3$ are three appropriate low Miller index microfacets;

a^i ($i=1, 2, 3$) are the vector decomposition coefficients of the vector

$(hk\ell)$ in terms of the three sets of microfacet indices $(h_i k_i \ell_i)$;

cf. Eqs. 13, 17 and 19; (when one of the coefficients a^i vanishes, the corresponding term in (1) may be dropped);

n_i^{uc} ($i=1, 2, 3$) are subscripts indicating the numbers of unit cells of each microfacet in the unit cell of the surface; cf. Eqs. 14-16, 18 and 20.

As will be demonstrated later, the coefficients a^i are obtained directly from the Miller indices (hke) of the surfaces, while the subscripts n_i^{uc} are simply related to the coefficients a^i (cf. Section 4.1).

For example, the Pt(10,8,7) surface would be described by (Pt has a fcc lattice)

$$Pt(S) = [7_{14}(111) + 1_1(110) + 2_2(100)]$$

or, alternatively, with other microfacets,

$$Pt(S) = [(\frac{15}{2})_{15}(111) + (\frac{1}{2})_1(11\bar{1}) + 2_2(100)].$$

Similarly, the Pt(775) surface is written as

$$Pt(S) = [5_5(111) + 2_1(110)]$$

and the Pt(755) surface is written as

$$Pt(S) = [5_5(111) + 2_1(100)].$$

With this notation, it is also easy to obtain the Miller indices from a known microfacet structure. From the numbers of microfacet unit cells n_i^{uc} one obtains directly the coefficients a^i and from these one can immediately produce the Miller indices by vectorial addition (cf. Section 8).

4. Relative Sizes of Microfacets on Surfaces of Three-dimensional Crystals.

The considerations of Section 2 generalize easily to the two-dimensional surfaces of three-dimensional cubic crystals. Thus, one may write $(110) = \frac{1}{2}(111) + \frac{1}{2}(11\bar{1})$, which means that a (110) unit cell can be regarded as being composed of a (111) and of a $(11\bar{1})$ microfacet, both of equal size. In general, the vector decompositions hold for any type of cubic lattices, but the interpretation in terms of number of unit cells of each microfacet depends on the lattice type.

Before entering into the detailed analysis of the microfacet decomposition of high Miller index crystal surfaces, it is necessary to point out a useful feature of the Miller indices: they can freely be scaled up or down without

changing their basic property (in cubic lattices) of being vectors perpendicular to the plane designated by the same indices (hkl) . We shall therefore in the following discussions freely scale the Miller indices to suitable integer values. However, in manipulating Miller indices one often obtains inconvenient values, such as $(\frac{1}{4}, 1, \frac{1}{2})$ or $(6, 10, 2)$ that one prefers to scale up or down to the set of smallest integers, such as (142) and (351) in the present examples. It must be stressed that some of the formulas that will be developed below require the use of the smallest set of integral indices: we call this the "irreducible" set of Miller indices.

4.1 Vector Decomposition of Miller Indices

To analyze and justify the vector decomposition in more detail, we consider an arbitrary surface characterized by the Miller index vector $\vec{u}_0 = (h_0 k_0 l_0)$, and decompose it into two microfacets characterized by the sets of Miller indices $\vec{u}_1$ and $\vec{u}_2$. (Each of these microfacets may in turn be decomposed into other microfacets, thereby providing a decomposition of the original surface into any number of microfacets.) The decomposition can thus be written in general as

$$\vec{u}_0 = a^1 \vec{u}_1 + a^2 \vec{u}_2.$$

Figure 2 shows the relationship between these vectors and the areas S of the surface unit cell and the areas F_1 and F_2 of the microfacets. (By surface unit cell we mean the repeating structural unit of the surface (hkl) : it typically includes a terrace and a step, but may be more complicated, namely with stepped surfaces.) Using the orthogonality of the vector (hkl) to the plane described by the Miller indices (hkl) , the similar triangles in Figure 2 yield the proportionalities

$$S:F_1:F_2 = |\vec{u}_0| : |a^1 \vec{u}_1| : |a^2 \vec{u}_2| \quad (2)$$

whereby the ratios between surface and microfacet areas are linked to the

decomposition coefficients a^1 and a^2 . It remains to relate these coefficients a^1 and a^2 to the unit cell areas A_0^{uc} , A_1^{uc} and A_2^{uc} of each surface or microfacet in order to obtain an easy comparison of the sizes of the microfacets.

In a simple cubic (sc) lattice, the area of the unit cell of an arbitrary surface defined by the Miller indices $(h,k,\ell)=u$ is

$$A_{sc}^{uc} = \sqrt{h^2+k^2+\ell^2} = |\vec{u}|. \quad (3)$$

This is because the product of that area and the interplanar spacing $d=(h^2+k^2+\ell^2)^{-1/2}$ should be the volume of the bulk unit cell, namely 1; we assume here, as implicit in the Miller index notation, that the lattice constant is 1. We have to assume here that the Miller indices are scaled to be the smallest possible integers. Similarly, for fcc lattices, the unit cell area is

$$A_{fcc}^{uc} = \begin{cases} \frac{\sqrt{h^2+k^2+\ell^2}}{2} = \frac{|\vec{u}|}{2} & \text{for } h,k,\ell \text{ not all odd} \\ \frac{\sqrt{h^2+k^2+\ell^2}}{4} = \frac{|\vec{u}|}{4} & \text{for } h,k,\ell \text{ all odd} \end{cases} \quad (4)$$

while for bcc lattices

$$A_{bcc}^{uc} = \begin{cases} \frac{\sqrt{h^2+k^2+\ell^2}}{2} = \frac{|\vec{u}|}{2} & \text{for } h+k+\ell = \text{odd} \\ \frac{\sqrt{h^2+k^2+\ell^2}}{4} = \frac{|\vec{u}|}{4} & \text{for } h+k+\ell = \text{even} \end{cases} \quad (5)$$

The denominators 2 and 4 in Eqs. 4 and 5 reflect the addition of face-centered and body-centered atoms; the microfacet unit cell area A_{sc}^{uc} for the simple cubic lattice can contain 1,2 or 4 atoms when face-centered or body-centered atoms are added.

It is now clear from Eq. 2 how the coefficients a^1 and a^2 should be interpreted to give the number of unit cells n_i^{uc} of each microfacet:

$$n_0^{uc} : n_1^{uc} : n_2^{uc} = \frac{|\vec{u}_0|}{A_0^{uc}} : a^1 \frac{|\vec{u}_1|}{A_1^{uc}} : a^2 \frac{|\vec{u}_2|}{A_2^{uc}} \quad (6)$$

the ratios $|u_i|/A_i^{uc}$ being 1, 2 or 4, depending on the faces used. Thus

$$n_0^{uc} : n_1^{uc} : n_2^{uc} = p_0 : a^1 p_1 : a^2 p_2 \quad (7)$$

where

$$p_i = \begin{cases} 1 & \text{for } \begin{cases} \text{sc lattices} \\ \text{bcc lattices, when } h_i + k_i + \ell_i = \text{odd} \end{cases} \\ 2 & \text{for } \begin{cases} \text{fcc lattices, when } h_i, k_i, \ell_i \text{ not all odd} \\ \text{bcc lattices, when } h_i + k_i + \ell_i = \text{even} \end{cases} \\ 4 & \text{for fcc lattices, when } h_i, k_i, \ell_i \text{ all odd.} \end{cases} \quad (8)$$

(Here, h, k, ℓ must be an irreducible set of integers; for fcc surfaces p_i is always even and one may divide all p_i 's by 2 in writing proportionalities such as in Eq.7.)

Equation 7 constitutes one of our main results: it tells us that p_0 unit cells of the surface $(hk\ell)$ contain $a^1 p_1$ unit cells of the microfacet $\vec{u}_1$ and $a^2 p_2$ unit cells of the microfacet $\vec{u}_2$. Thus one unit cell of the surface $(hk\ell)$ contains $a^1 p_1/p_0$ and $a^2 p_2/p_0$ unit cells of the microfacets $\vec{u}_1$ and $\vec{u}_2$, respectively.

As mentioned before, one may further decompose individual microfacets into other microfacets. Thus with altogether three microfacets, an arbitrary surface $\vec{u}_0 = (hk\ell)$ decomposes as

$$\vec{u}_0 = a^1 \vec{u}_1 + a^2 \vec{u}_2 + a^3 \vec{u}_3 \quad (9)$$

and Eq. 7 will take the form

$$n_0^{uc} : n_1^{uc} : n_2^{uc} : n_3^{uc} = p_0 : a^1 p_1 : a^2 p_2 : a^3 p_3 \quad (10)$$

with p_i as in Eq.8. This is of particular significance for surfaces of three-dimensional crystals: one knows that vectors can be decomposed uniquely onto a basis set of three linearly independent vectors, and therefore it follows that

an arbitrary surface can be decomposed uniquely in terms of three microfacets with linearly independent Miller indices. The three microfacets $\vec{u}_1$, $\vec{u}_2$ and $\vec{u}_3$ contain, respectively, $a^1 p_1/p_0$, $a^2 p_2/p_2$ and $a^3 p_3/p_0$ unit cells. Our microfacet notation (cf. Eq.1) contains these numbers (called n_i^{uc} there) and the coefficients a^1, a^2, a^3 . A general method for obtaining the decomposition coefficients a_i of $\vec{u}_0$ onto the microfacets $\vec{u}_i$ ($i=1,2,3$) is provided by the Cramer relations (which apply for arbitrary linearly independent vectors $\vec{u}_i$):

$$a^1 = \frac{(\vec{u}_0, \vec{u}_2, \vec{u}_3)}{(\vec{u}_1, \vec{u}_2, \vec{u}_3)} \quad a^2 = \frac{(\vec{u}_1, \vec{u}_0, \vec{u}_3)}{(\vec{u}_1, \vec{u}_2, \vec{u}_3)} \quad a^3 = \frac{(\vec{u}_1, \vec{u}_2, \vec{u}_0)}{(\vec{u}_1, \vec{u}_2, \vec{u}_3)} \quad (11)$$

where the mixed product is used:

$$(\vec{a}, \vec{b}, \vec{c}) = \vec{a} \cdot (\vec{b} \times \vec{c}). \quad (12)$$

3.2 Low Miller Index Microfacets

We now apply Eqs. 9 and 10 to the decomposition of surfaces of sc, fcc and bcc lattices in terms of low-Miller-index microfacets. It is often convenient to consider microfacets of (111), (110) and (100) orientation. If we further choose for convenience (without loss of generality) to order the Miller indices (hkl) in such a way that $h \geq k \geq l$, then

$$(hkl) = l(111) + (k-l)(110) + (h-k)(100), \quad (13)$$

which yields for the number of unit cells:

$$n_{hkl}^{uc} : n_{111}^{uc} : n_{110}^{uc} : n_{100}^{uc} = \begin{cases} p_{hkl}^{sc} : l : k-l : h-k & \text{for sc} \\ p_{hkl}^{fcc} : 4l : 2(k-l) : 2(h-k) & \text{for fcc} \\ p_{hkl}^{bcc} : l : 2(k-l) : h-k & \text{for bcc} \end{cases} \quad (14)$$

$$(15)$$

$$(16)$$

where p is defined in Eq. 8 (for the microfacet notation of Section 3, these numbers are normalized to $n_{hke}^{uc}=1$). One may prefer not to use (110) microfacets for surfaces of fcc materials, since they are not close packed, but rather (111), (11 $\bar{1}$) and (100) microfacets. This is simply achieved by decomposing Eq. 13 further with $(110)=\frac{1}{2}(111) + \frac{1}{2}(11\bar{1})$, yielding

$$(hke) = \frac{k+l}{2}(111) + \frac{k-l}{2}(11\bar{1}) + (h-k)(100) \quad (17)$$

and

$$n_{hke}^{uc} : n_{111}^{uc} : n_{11\bar{1}}^{uc} : n_{hke}^{uc} = p_{hke}^{fcc} : 2(k+l) : 2(k-l) : 2(h-k) \quad \text{for fcc} \quad (18)$$

With bcc surfaces a decomposition according to (110), (100) and (001) microfacets may be more convenient, since bcc (111) is not a close-packed face. With $h \geq k$ we get then

$$(hki) = k(110) + (h-k)(100) + l(001) \quad (19)$$

and therefore

$$n_{hke}^{uc} : n_{110}^{uc} : n_{100}^{uc} : n_{001}^{uc} = p_{hke}^{bcc} : 2k : h-k : l \quad \text{for bcc} \quad (20)$$

The resulting microfacet notation, together with the step notation, is illustrated in Table 1 for surfaces of fcc crystals.

We now give examples of these decompositions. An elementary case for the fcc surfaces is the decomposition of a (110) face into its microfacets:

$$(110) = \frac{1}{2}(111) + \frac{1}{2}(11\bar{1}). \quad \text{This yields from Eq. 18}$$

$$n_{110}^{uc} : n_{111}^{uc} : n_{11\bar{1}}^{uc} = 2 : 2 : 2 = 1 : 1 : 1,$$

and with the microfacet notation:

$$fcc(110) = fcc(S) - \left[\left(\frac{1}{2}\right)_1(111) + \left(\frac{1}{2}\right)_1(11\bar{1})\right]$$

Figure 3 illustrates this decomposition and shows how, for each (110) unit cell, the (111) and (11 $\bar{1}$) microfacets contain one unit cell each.

A surface with a typical step structure is illustrated in Figure 4.

This fcc (775) surface decomposes as

$$\begin{aligned}(775) &= 5(111) + 2(110) \\ &= 6(111) + (11\bar{1}),\end{aligned}$$

yielding from Eqs. 15 and 18:

$$\begin{aligned}n_{775}^{uc} : n_{111}^{uc} : n_{11\bar{1}}^{uc} : n_{110}^{uc} &= 4:20:0:4 = 1:5:0:1 \\ \text{or} \quad 4:24:4:0 &= 1:6:1:0,\end{aligned}$$

respectively. These ratios can be recognized in Figure 4. The microfacet notation is:

$$\begin{aligned}\text{fcc}(775) &= \text{fcc}(S) - [5_5(111) + 2_1(110)] \\ &= \text{fcc}(S) - [6_6(111) + 1_1(11\bar{1})].\end{aligned}$$

The fact that some numbers n_i^{uc} are zero indicates that we have a non-kinked surface.

For comparison we illustrate the fcc(755) surface in Figure 5. It decomposes as

$$(755) = 5(111) + 2(100),$$

so that, from Eq.15:

$$n_{755}^{uc} : n_{111}^{uc} : n_{100}^{uc} = 4:20:4 = 1:5:1,$$

and in microfacet notation:

$$\text{fcc}(755) = \text{fcc}(S) - [5_5(111) + 2_1(100)].$$

This is also a non-kinked surface. Note the similar terrace, (111), but different step, (100) vs. (110) or (11 $\bar{1}$) of the (755) surface as compared with the (775) surface.

The fcc (10,8,7) surface is an example of a kinked surface and is shown in Figure 6. This surface decomposes as

$$\begin{aligned}(10,8,7) &= 7(111) + (310) \\ &= 7(111) + (110) + 2(100) \\ &= \frac{15}{2}(111) + \frac{1}{2}(11\bar{1}) + 2(100),\end{aligned}$$

and we obtain the following ratios of numbers of unit cells:

$$n_{10,8,7}^{uc} : n_{111}^{uc} : n_{310}^{uc} = 2:28:2 = 1:14:1$$

$$\begin{aligned} n_{10,8,7}^{uc} : n_{111}^{uc} : n_{11\bar{1}}^{uc} : n_{110}^{uc} : n_{100}^{uc} &= 2:28:0:2:4 = 1:14:0:1:2 \\ &= 2:30:2:0:4 = 1:15:1:0:2 \end{aligned}$$

The microfacet notation gives:

$$\begin{aligned} fcc(10,8,7) &= fcc(S) - [7_{14}(111) + 1_1(310)] \\ &= fcc(S) - [7_{14}(111) + 1_1(110) + 2_2(100)] \\ &= fcc(S) - \left[\left(\frac{15}{2}\right)_{15}(111) + \left(\frac{1}{2}\right)_1(11\bar{1}) + 2_2(100) \right]. \end{aligned}$$

We see quite clearly that the terraces have a (111) orientation and we can visualize the step structure as well; the steps of (310) orientation are composed of (100) and 2(100) microfacets. Alternatively, thinking in terms of (111), (11 $\bar{1}$) and (100) microfacets, the above decomposition shows that

$$(10,8,7) = \frac{15}{2} (111) + \frac{5}{2} (51\bar{1}).$$

In these terms the steps have a (51 $\bar{1}$) orientation, as is also visible in Fig.6; these steps are composed of one unit cell of (11 $\bar{1}$) microfacet and two unit cells of (100) microfacet.

However, it is not obvious from the above ratios how two successive steps are positioned with respect to each other; especially their relative position in the direction parallel to the steps is not clear. Without additional information it would be difficult to visualize the surface structure unless one adopts a trial-and-error method, shifting successive steps with respect to each other until the terrace has exactly the required area. Section 5 will help in providing additional information for this purpose.

4. Terraces, steps and kinks

The numbers of unit cells of each microfacet, as given by Eqs. 9 and 10, enable us to identify which of the microfacets is the terrace and allow the determination of the numbers of terrace atoms, step atoms and kink atoms. The terrace is simply that microfacet which has the largest number of unit cells n_i^{uc} . Thus the fcc(755) surface has $n_{111}^{uc}:n_{11\bar{1}}^{uc}:n_{100}^{uc}=5:0:1$, and therefore the (111) microfacet is the terrace, with 5 times as many atoms as the (100) microfacet, cf. Figure 5.

If two of the number n_i^{uc} are equal and largest, the surface is composed of two equal length one-atom wide terraces of different orientation, interrupted by single-atom microfacets of the third orientation at regular intervals. For example, a fcc(11,10,1) surface decomposes as $5(111)+5(11\bar{1})+(100)$, exhibiting 10-atom-long (111) and (11 $\bar{1}$) terraces, i.e. a stretch of (110) surface, interrupted by (100) microfacets representing the start of new rows of atoms in the troughs of the (100) surface; we thus have a stepped (110) surface with step edges perpendicular to the troughs.

Given the relative numbers of unit cells of each microfacet, one can easily find the ratio between the different types of surface atoms; terrace atoms, step atoms (including kink atoms or not) and kink atoms alone (those atoms sticking most out of the surface, i.e. those atoms with the fewest nearest neighbors). Starting with Eq.10, the three decomposition coefficients n_i^{uc} ($i=1,2,3$) are re-named n_{min} , n_{mid} and n_{max} according to their relative size; these three numbers then are proportional to the numbers of kink atoms, non-kink step atoms and terrace atoms, respectively. Therefore, the following ratios hold for the numbers of different types of atoms:

$$\text{kink atoms} : \text{non-kink step atoms} : \text{all step atoms} : \text{terrace atoms} : \text{all atoms} =$$

$$n_{\min} : n_{\text{mid}} : n_{\min} + n_{\text{mid}} : n_{\max} : n_{\min} + n_{\text{mid}} + n_{\max} \quad (21)$$

As an example, we apply Eq. 21 to the fcc(10,8,7) surface, assuming (111), (110) and (100) microfacets:

$$\begin{aligned} \text{Kink atoms} : \text{non-kink step atoms} : \text{all step atoms} : \text{terrace atoms} : \\ \text{all atoms} = 1 : 2 : 3 : 14 : 17. \end{aligned}$$

These numbers can be easily recognized in Figure 6.

One can of course also obtain absolute surface concentrations of atoms of any type. For this purpose the above numbers must be normalized to one unit cell of the macroscopic surface and divided by the area of that unit cell. From Eq. 10 we **must** use $n_{\min}/n_o^{\text{uc}}$, $n_{\text{mid}}/n_o^{\text{uc}}$ and $n_{\max}/n_o^{\text{uc}}$ which are respectively the numbers of kink atoms, step atoms and terrace atoms, so that for example

$$\text{kink atom density} = (n_{\min}/n_o^{\text{uc}})/(|\vec{u}_o|/p_o). \quad (22)$$

Here, the unit for the area is the cube edge squared.

Once the terrace orientation $(h_t k_t \ell_t)$ has been identified, it is simple to find the Miller indices $(h_s k_s \ell_s)$ of the step itself. If a_t was the decomposition coefficient in Eq. 9 for the terrace, then

$$(h_s k_s \ell_s) = (h k \ell) - a_t (h_t k_t \ell_t) \quad (23).$$

(if the indices h_s , k_s , ℓ_s are not all integers, they should be scaled up to yield integers). Frequently, this step $(h_s k_s \ell_s)$ is a not-so-high Miller index microfacet which one likes to identify as such for comparison with identical or similar steps on other surfaces.

5. The surface structure

Even with the knowledge obtained in Section 3 about the sizes of the microfacets composing a surface, it is only possible to visualize the surface structure in the simpler cases. Thus one can readily picture the (755) surface

composed of 5-atom wide (111) terraces and single height (100) steps. But the (10,8,7) is not easily pictured without additional information. The most important such information is the shape and orientation of the surface unit cell; this will be determined in this Section by giving the two basis vectors of the repeating surface structure. Further useful information given in this Section include inclination angles and the surface reciprocal lattice.

One type of information that can be easily obtained about surfaces labelled by their Miller indices is the angle between two planes of interest. Thus the angle α_i between the surface plane $\vec{u}_0$ and any microfacet $\vec{u}_i$ is given by the familiar formula

$$\cos \alpha_i = \frac{\vec{u}_0 \cdot \vec{u}_i}{|\vec{u}_0| |\vec{u}_i|} \quad (24)$$

The terrace width is now also easily determined, once we know the step height d_i for the microfacet $\vec{u}_i$; d_i is just the layer spacing between planes perpendicular to u_i (cf. Eq.3 for the case of simple cubic materials):

$$d_i = \frac{1}{q_i} \frac{1}{|\vec{u}_i|} \quad (25)$$

where

$$q_i = \begin{cases} 1 & \begin{cases} \text{for sc} \\ \text{for fcc with } h_i, k_i, \ell_i \text{ all odd} \\ \text{for bcc with } h_i + k_i + \ell_i = \text{even} \end{cases} \\ 2 & \begin{cases} \text{for fcc with } h_i, k_i, \ell_i \text{ not all odd} \\ \text{for bcc with } h_i + k_i + \ell_i = \text{odd} \end{cases} \end{cases} \quad (26)$$

(the numbers q_i take the addition of centered atoms to the simple cubic lattice into account). Now the terrace width w_t measured parallel to the terrace plane is

$$w_t = \frac{d_i}{\tan \alpha_i} \quad (27)$$

with α_i given by Eq.24. This terrace width w_t is defined as the projection onto the terrace plane of the repeat distance w_s along the macroscopic surface, perpendicular to the terrace edges; thus w_s is the shortest distance from one terrace edge to the next, namely

$$w_s = \frac{d_i}{\sin \alpha_i} \quad (28)$$

We now construct a vector $\vec{e}$ that describes the edge of the terrace; $\vec{e}$ is parallel to the terrace edge and has a length such that it points from one atom on the edge to the next equivalent atom (e.g. from one kink atom to the next equivalent kink atom along the edge). This vector is one of the two basis vectors $\vec{e}$ and $\vec{w}$ describing the unit cell of the surface structure. Its direction is simply given by the cross product of the surface normal $\vec{u}_0$ and the terrace normal $\vec{u}_t$. Its length must be such that the surface unit cell has the proper area, i.e. $|\vec{e}| w_s = |\vec{u}_0|/p_0$, according to Eqs. 3-5, 8 and 28. It follows that

$$\vec{e} = \pm \frac{q_t}{p_0} \vec{u}_t \times \vec{u}_0 \quad (29)$$

To construct the second basis vector $\vec{w}$ of the surface unit cell, a vector which relates one step to the next, we start by finding a surface lattice vector in the following manner. The vector $\vec{w}' = \vec{u}_0 \times \vec{e}$ is a lattice vector in the surface plane and perpendicular to $\vec{e}$, i.e. it has roughly the correct direction to relate one step to the next, but it requires proper adjustments in length and direction (within the surface plane). The vector $\vec{w}'$ is normally too large to be a basis vector and must first be scaled down to $\omega \vec{w}'$ by the requirement that the unit cell area $|\omega \vec{w}' \times \vec{e}| = |\vec{u}_0|/p_0$ be obtained, or by the equivalent requirement that $\omega \vec{w}'$ give the proper step height, i.e. $|\omega \vec{w}' \cdot \vec{u}_t|/|\vec{u}_t| = n_s d_t$, where n_s is the number of steps contained in one surface unit cell, i.e. n_{mid}/n_o^{uc} (cf. Section 4;

$n_s=1$ except for stepped surfaces, etc.). However, not every lattice vector when scaled down yields another lattice vector, but $\vec{w}' + m\vec{e}$ for a suitable finite integer m will satisfy that requirement. Thus the procedure for constructing the basis vector $\vec{w} = \omega(\vec{w}' + m\vec{e})$ is to make this vector satisfy one of the two above requirements (this fixes ω , but not m) and to scan through a finite number of values of m until a lattice vector is obtained (the number of scanned values of m will be at most $1/\omega$).

Thus the surface basis vectors $\vec{e}$ and $\vec{w}$ have been determined. From these we can easily generate the two-dimensional reciprocal lattice of the macroscopic surface for comparison with Low Energy Electron Diffraction patterns. Using $\vec{u}_0 = (hk\ell)$ as the surface normal, the two-dimensional reciprocal lattice of the surface has the following basis vectors:

$$\vec{e}^* = 2\pi \frac{\vec{w} \times \vec{u}_0}{\vec{e} \cdot (\vec{w} \times \vec{u}_0)}, \quad \vec{w}^* = 2\pi \frac{\vec{u}_0 \times \vec{e}}{\vec{e} \cdot (\vec{w} \times \vec{u}_0)}. \quad (30)$$

Here $\vec{w}^*$ is perpendicular to the step edges and therefore gives the "spot splitting" often observed in LEED patterns for stepped and kinked surfaces; $\vec{e}^*$ does not in general have a simple direction (it is perpendicular to $\vec{w}$, however).

It is often helpful to express the various vectors of interest in terms of basis vectors within the individual microfacets, such as the simple interatomic vectors within the (100) or (111) faces. In general, the natural choice for these basis vectors is the set of three vectors $\vec{b}_i$ that are parallel to the three lines of intersection between the three microfacets under consideration, cf. Fig.7. We shall give these a length such that they point from one atom to the next on the three edges so defined. (A kink atom can be considered to be at the apex of a pyramid whose faces are three microfacets joining at three edges,

cf. Fig.7 ; our basis vectors will point along these three edges), Eq. 29 provides such vectors by simple extension. If $\vec{u}_1, \vec{u}_2$ and $\vec{u}_3$ are the microfacet normals, then

$$\vec{b}_1 = \pm \frac{q_2}{p_3} \vec{u}_2 \times \vec{u}_3, \quad \vec{b}_2 = \pm \frac{q_3}{p_1} \vec{u}_3 \times \vec{u}_1, \quad \vec{b}_3 = \pm \frac{q_1}{p_2} \vec{u}_1 \times \vec{u}_2. \quad (31)$$

The signs might be chosen so as to make each $\vec{b}_i$ point into the surface, when possible. Any vector can now be decomposed onto $\vec{b}_1, \vec{b}_2$ and $\vec{b}_3$ by applying the Cramer relations of Eq.11.

Our results can be easily programmed for a computer to produce useful information about many arbitrary surfaces for comparison of their properties. We shall tabulate some of these results in Section 8.

It remains to put together the various pieces of information obtained above to construct the surface. We find that the easiest procedure for doing this consists of first drawing a portion of an infinite terrace and then erecting the step components on this terrace so that they join properly and produce the terrace edge vector $\vec{e}$ of Eq. 29. With fcc materials, for a (111) terrace any (100) squares of a step face have to fit with two corners on two terrace atoms, and likewise for the (110) rectangles of a step face, where the short side of the rectangle fits on the terrace. This is seen in Figs. 4-6. For a (100) terrace any (111) parallelograms fit with two corners on two terrace atoms, and likewise for the (110) rectangles of a step face, where the long side of the rectangle fits on the terraces. Note that microfacets do not necessarily have simple shapes. For example a (100) microfacet need not be a simple juxtaposition of squares; it may be a parallelogram or also have an irregular contour with concave parts. See Fig.6, for examples.

Once a step has been assembled, successive steps are simply obtained

by translation through the terrace width vector $\vec{w}$ defined above, and thereby the surface structure is determined. However, for stepped surfaces, (cf. Fig.1b and the discussion in Section 7) one has to be careful to split some microfacets into disjoint parts of unequal size. The general guideline for doing this is to assemble a surface that best approximates a plane perpendicular to the $(hk\ell)$ vector.

6. Surfaces of other types of material

All cubic lattices besides the simple cubic, face-centered cubic and body-centered cubic lattices can also be treated exactly as described in the preceding sections. Thus the diamond structure consists of an fcc lattice with two identical atoms in each unit cell. A surface given by Miller indices $(hk\ell)$ will have the same microfacet structure as the $(hk\ell)$ surface of a face-centered cubic material. The only difference concerns the question of the termination of the surface in such cases (i.e. which of the two atoms in the three-dimensional unit cell becomes the surface atom); this is a physical problem unrelated to the geometrical decomposition into microfacets (we, of course, exclude reconstructions and facetting from these considerations). Similarly, the zincblende structure and the sodium chloride structure are also face-centered cubic structures with two (unidentical) atoms in each unit cell. And the cesium chloride structure is a simple cubic structure with two (unidentical) atoms in each unit cell. For all these cubic lattices, the results of the preceding sections can be applied directly, one only needs to imagine that each atom in those results is replaced by a pair of atoms.

Non-cubic crystals (such as hexagonal-close packed and wurtzite crystals)

require a more complicated analysis. The reason is that we have used as our starting point the orthogonality between a plane with Miller indices $(hk\ell)$ and the vector $(hk\ell)$ itself (cf. Eq.2). This orthogonality only holds for cubic lattices.

7. Classes of surfaces

The decomposition described in Sections 3 and 4 for arbitrary surfaces of cubic materials enables one to classify surfaces by common characteristics. Thus one may consider the surfaces that have no kinks, i.e. the surfaces for which one of the three decomposition coefficients vanishes. For example, using Eqs. 13 and 15 fcc $(hk\ell)$ surfaces with $k=\ell$ have only the microfacets (111) and (100) and therefore have no kinks. An example is fcc (755) , illustrated in Fig.5. Surfaces with $h=k$ similarly have no (100) microfacets and no kinks. An example is fcc (775) , shown in Fig.4. And when $\ell=0$, only (110) and (100) microfacets occur with no kinks (the (110) microfacets may still be considered to be composed of a mosaic of (111) and $(11\bar{1})$ microfacets, of course). An extreme example is the fcc (110) surface itself, cf. Fig.3.

One may also consider the class of all surfaces $(hk\ell)$ that have a common step orientation $(h_s k_s \ell_s)$, but variably-sized terraces of fixed orientation $(h_t k_t \ell_t)$. These surfaces are then simply given by

$$(hk\ell) = (h_s k_s \ell_s) + m_t (h_t k_t \ell_t) \quad (32)$$

where the arbitrary integer m_t represents the size of the terrace and is related to the number of unit cells on the terrace by Eq.10. This is also the family of surfaces with a constant ratio of number of kink atoms to other step atoms. Thus, the $(10,8,7)$ surface has (310) steps (with $m_t=7$) and thus a 2:1

ratio of kink atoms to other step atoms; and so do the (976) and (865) surfaces (with $m_t=6$ and 5, respectively).

One may generate a class of fixed terrace size but variable step structure. This can be done by using Eq.21. If we require, for example, different surfaces with a constant density of step atoms, we obtain the condition

$$\frac{n_{\min} + n_{\text{mid}}}{n_{\min} + n_{\text{mid}} + n_{\max}} = \text{constant.} \quad (33)$$

Given a value α for the constant (such as the value appropriate for one given surface), it follows that

$$n_{\min} + n_{\text{mid}} = \frac{\alpha}{1-\alpha} n_{\max} \quad (34)$$

must be satisfied. Thus we may try to find different surfaces with the same step atom density as the fcc(755) surface. This fixes $\alpha=1/6$, so that Eq.34 becomes $n_{\min} + n_{\text{mid}} = \frac{1}{5} n_{\max}$. Thus $n_{\max}$ must be a multiple of 5. The simpler inequivalent solutions of this equation are

$$(n_{\max}, n_{\text{mid}}, n_{\min}) = (510), (10,1,1), (15,2,1), \overset{(20,3,1),}{(25,4,1)} (25,3,2), \text{ etc.}$$

yielding fcc surfaces with Miller indices

$$(755), (13,11,9), (10,8,7), (27,21,19), (17,13,12), (33,27,23), (332),$$

$$(19,17,13), (25,23,17), (31,29,21), (16,14,11), \text{ etc. [these results are}$$

based on (111), (11 $\bar{1}$) and (100) microfacets, the first six correlating $n_{\min}$ with (11 $\bar{1}$) and the last five correlating $n_{\min}$ with (100); this transition from numbers of unit cells to Miller indices will be explained more fully in the next section].

We now consider the large class of stepped stepped surfaces, of which the (2,5) surface in Section 2 was a prototype. The fcc(411) surface also

belongs to this class; clearly, then, such surfaces need not have very high Miller indices, nor do they necessarily have very large surface unit cells.

With our description in terms of microfacets, this class subdivides into three subclasses: the first, which we call "variable-terrace surfaces", has successive terraces of unequal sizes (as in the (2,5) surface of Section 2); the second, which we call "variable-kink surfaces", has step faces that can be thought to consist of unequal successive terraces (i.e. the kink atoms are not evenly spaced along the step and are therefore not all equivalent); the third subclass, which we call "variable-terrace-and-kink surfaces", combines both features simultaneously. Thus the fcc (411) surface decomposes as

$$(411) = 3(100) + (111);$$

it is not kinked with

$$n_{100}^{uc} : n_{111}^{uc} = 3 : 2.$$

None of the integers of this ratio can be reduced to 1, so that we have a stepped stepped surface. Its surface unit cell contains two (100) terraces of 2 and 1 unit cells, respectively ($2 + 1 = n_{100}^{uc}$) separated by two (111) steps of one unit cell each ($1 + 1 = n_{111}^{uc}$). This is a variable-terrace surface, which in projection would have an appearance similar to Fig.2b.

We can build a surface of the second kind (variable-kink surface) by using (411) as the step face on a surface with (11 $\bar{1}$) terraces, e.g. (retaining fcc lattices)

$$(96\bar{4}) = (411) + 5(11\bar{1}) = 3(100) + (111) + 5(11\bar{1})$$

which yields

$$n_{411}^{uc} : n_{11\bar{1}}^{uc} = 1 : 10.$$

Since one of these integers is 1, this is not a variable-terrace surface, and thus only a variable-kink surface. Its appearance can be imagined by considering

Fig.2b to represent one step edge viewed perpendicularly to the terrace plane:

The following combination of (411) and $(11\bar{1})$ produces a variable-terrace-and-kink surface

$$(17,8,\bar{2}) = 3(411) + 5(11\bar{1}) = 9(100) + 3(111) + 5(11\bar{1}),$$

since

$$n_{411}^{uc} : n_{11\bar{1}}^{uc} = 3 : 10$$

cannot be reduced to produce an integer of 1. This surface has three unequal terraces in the repeating unit and the steps have unequally spaced kink atoms.

Generally speaking, if $(hk\ell)$ consists of a terrace $(h_t k_t \ell_t)$ and a step $(h_s k_s \ell_s)$, which in turn consists of microfacets $(h_{s1} k_{s1} \ell_{s1})$ and $(h_{s2} k_{s2} \ell_{s2})$ we may write the decomposition as

$$\begin{aligned} (hk\ell) &= a^t (h_t k_t \ell_t) + a^s (h_s k_s \ell_s) \\ &= a^t (h_t k_t \ell_t) + a^{s1} (h_{s1} k_{s1} \ell_{s1}) + a^{s2} (h_{s2} k_{s2} \ell_{s2}). \end{aligned}$$

The coefficients lead to the following relevant ratios of numbers of unit cells (we assume these ratios to be put in their irreducible form, i.e. written as the smallest possible integers):

$$\begin{aligned} n_t^{uc} : n_s^{uc} &= p_t a^t : p_s a^s \\ n_{s1}^{uc} : n_{s2}^{uc} &= p_{s1} a^{s1} : p_{s2} a^{s2}. \end{aligned}$$

If the first of these ratios contains an integer 1, but the second does not, we have a variable-terrace surface; if the second ratio contains an integer 1, but the first does not, we have a variable-kink surface; and if neither ratio contains an integer 1, we have a variable-terrace-and-kink surface.

8. Determination of the Miller indices from the surface structure

So far we have concentrated on the problem of finding the structure of

an arbitrary surface $(hk\ell)$. The inverse problem consists of determining the Miller indices $(hk\ell)$ from structural information. One frequently wishes to perform experiments on surfaces with a particular terrace orientation and a particular step density and/or kink density, and perhaps with a given step orientation. For example, one may wish to find a stepped fcc surface with (111) terraces, (100) steps and a step-to-terrace atom ratio of 1:5. Which are the Miller indices of the surface that satisfies these requirements?

This kind of question is easily solved by using Eq.10 with Eq.8. (ignoring n_o^{uc} and p_o) to determine a^1, a^2 and a^3 , and then summing $a^1 u_1 + a^2 u_2 + a^3 u_3 = (hk\ell)$. Thus for the above example, one may write, from Eq.10,

$$n_{111}^{uc} : n_{11\bar{1}}^{uc} : n_{100}^{uc} = 5:0:1 = 4a^1 : 4a^2 : 2a^3,$$

which implies $(a^1, a^2, a^3) = (\frac{5}{4}, 0, \frac{1}{2}) \propto (5, 0, 2)$ and so by vector addition

$$(hk\ell) = 5(111) + 0(11\bar{1}) + 2(100) = (755).$$

Although the foregoing reasoning is simple, we include for convenience in Table II a list of results that can help in finding rapidly a non-kinked fcc surface with desired characteristics.

A different problem is the determination of the Miller indices of a surface from an observed LEED pattern for that surface. The general solution would consist of three parts: measure the reciprocal lattice from the LEED pattern invert it to obtain the surface unit cell and then find which Miller indices correspond to that unit cell. However, the first and third of these parts are difficult. The first part suffers from the fact that usually most diffraction spots are too weak to be detected. Only those spots close to the positions of the spots for the non-stepped terrace are usually detectable; these are the well-known "split spots", which are really only a few of the many step superlattice spots that one expects in principle, cf. Fig.7. The

undetectability of many spots makes the measurement of the reciprocal lattice quite imprecise, especially as the spots are usually not extremely sharp and the pattern is usually somewhat distorted in the electron optics and in the photography of the diffraction pattern. The third part, that of obtaining the Miller indices from a given surface unit cell, is difficult, especially when experimental uncertainties are taken into account, because we do not have a simple invertible relation between the surface basis vectors $\vec{e}$ and $\vec{w}$ spanning the unit cell (cf. Section 5) on the one hand, the the Miller indices $(hk\ell)$ on the other hand.

In practice one can more conveniently find the crystal surface orientation by combining X-ray diffraction (to determine the bulk orientation) and laser reflection (to determine the surface orientation relative to the bulk). However, LEED can still be used to at least check the result by comparing calculated quantities with some easily measured features of the LEED pattern. These features could be the spot-splitting distance and the distance between nearest rows of split spots; these distances are shown in Fig.7 for the case of the fcc (10,8,7) surface, where they are called b and a , respectively. Their ratio also is included in Table II for some fcc surfaces (this ratio provides the generalization to arbitrary cubic surfaces of the spot-splitting formulas of Henzler⁵).

Acknowledgements

We wish to thank S.M. Davis for fruitful discussions and very helpful suggestions.

This work was supported by the Division of Materials Sciences, Office of Basic Energy Sciences, U.S. Department of Energy. Prepared for the U.S. Department of Energy under contract No. S-7405-Eng-48.

References:

1. J.K. Mackenzie, A.J.W. Moore and J.F. Nicholas, J. Phys. Chem. Solids 23, 185 (1962);
J.K. Mackenzie and J.F. Nicholas, J. Phys. Chem. Solids, 23
197 (1962).
2. J.F. Nicholas, "An Atlas of Models of Crystal Surfaces", Gordon and Breach (New York) 1965.
3. B. Lang, R.W. Joyner and G.A. Somorjai, Surface Sci. 30, 454 (1972).
4. C. Kittel, "Introduction to Solid State Physics", Wiley (New York) 1966, 3rd ed. pp. 44 and 56.
5. M. Henzler, Surface Sci. 19, 159 (1970).

Table Captions

Table I: List of surfaces of fcc crystals, giving the Miller indices, the microfacet notation and the step notation. These surfaces correspond to those in Table II (omiting stepped stepped surfaces). The step notation gives the number of atoms across a terrace, including the first and last ones; this number is larger by one than the number of unit cells across a terrace, as used in the microfacet notation. In addition, for kinked surfaces, such as the $(n+3, n+1, n)$ family, the step notation still only counts as one row of atoms across the terrace; whereas the microfacet notation counts all terrace unit cells that fit inside the unit cell of the macroscopic surface, i.e. the microfacet notation counts not only across the terrace, but also along it.

Table I.

(hkl)	microfacet notation	step notation
(n+1, n+1, n-1)	$n_n(111) + 1_1(11\bar{1})$	$(n+1)(111)x(111)$
(110)	$(\frac{1}{2})_1(111) + (\frac{1}{2})_1(11\bar{1})$	$2(111) \times (111)$
(331)	$2_2(111) + 1_1(11\bar{1})$	$3(111) \times (111)$
(221)	$(\frac{3}{2})_3(111) + (\frac{1}{2})_1(11\bar{1})$	$4(111) \times (111)$
(n+2, n, n)	$n_n(111) + 2_1(100)$	$(n+1)(111)x(100)$
(311)	$1_1(111) + 2_1(100)$	$2(111)x(100)$ or $2(100)x(111)$
(211)	$1_2(111) + 1_1(100)$	$3(111) \times (100)$
(533)	$3_3(111) + 2_1(100)$	$4(111) \times (100)$
(n+3, n+1, n)	$n_{2n}(111)+1_1(310)$	$n(111) \times (310)$
(421)	$1_2(111) + 1_1(310)$	$1(111) \times (310)$
(532)	$2_4(111) + 1_1(310)$	$2(111) \times (310)$
(643)	$3_6(111) + 1_1(310)$	$3(111) \times (310)$
(2n+1, 1, -1)	$2n_n(100) + 1_1(11\bar{1})$	$(n+1)(100)x(111)$
(3, 1, -1)	$2_1(100) + 1_1(11\bar{1})$	$2(100)x(111)$ or $2(111)x(100)$
(5, 1, -1)	$4_2(100)+1_1(11\bar{1})$	$3(100) \times (111)$
(n+1, 1, 0)	$n_n(100) + 1_1(110)$	$(n+1)(100)x(110)$
(210)	$1_1(100) + 1_1(110)$	$2(100) \times (110)$ or $2(110)x(100)$
(310)	$2_2(100) + 1_1(110)$	$3(100) \times (110)$
(410)	$3_3(100) + 1_1(110)$	$4(100) \times (110)$

(continued)

Table I (continued)

(hkl)	microfacet notation	step notation
(2n+1, 2n+1,1)	$2n_n(110) + 1_1(111)$	$(n+1)(110)x(111)$
(331)	$2_1(110) + 1_1(111)$	$2(110) \times (111)$
(551)	$4_2(110) + 1_1(111)$	$3(110) \times (111)$
(771)	$6_3(110) + 1_1(111)$	$4(110) \times (111)$
(n+1,n,0)	$n_n(110) + 1_1(100)$	$(n+1)(110)x(100)$
(210)	$1_1(110) + 1_1(100)$	$2(110) \times (100)$ or $2(100) \times (110)$
(320)	$2_2(110) + 1_1(100)$	$3(110) \times (100)$
(430)	$3_3(110) + 1_1(100)$	$4(110) \times (100)$

Table II: Properties are listed for high Miller index surfaces of fcc crystals. The surfaces are groups in classes (a)-(g) with common terrace and step orientation. For each class are indicated: the terrace orientation; the basis vectors (Eq.31) used for expressing the terrace edge and width vectors; the microfacet orientations used in the decomposition.

For each surface are given: the algebraic microfacet decomposition and the number of unit cells for each microfacet (these numbers are used in the microfacet notation of Section 3); the step orientation; the relative numbers of kink atoms, non-kink step atoms, terrace atoms and all surface atoms; the terrace edge and width vectors $\vec{e}$ and $\vec{w}$ (defining the surface unit cell), in cartesian coordinates and in terms of the basis vectors given at the top of each class (the unit of length is the cube edge), together with their lengths and the angle between them (this angle also appears in the LEED pattern between the rows of spots); the LEED spot splitting in units of 2π divided by the cube edge; the ratio of the spacing between nearest rows of split spots (measured perpendicular to the splitting direction) to the spot splitting.

The classes of surfaces are characterized by:

- a. (111) terraces with (11 $\bar{1}$) steps
- b. (111) terraces with (100) steps (excluding stepped stepped surfaces)
- c. (111) terraces with (310) steps
- d. (100) terraces with (11 $\bar{1}$) steps (including some stepped stepped surfaces.
- e. (100) terraces with (110) steps
- f. (110) terraces with (111) steps (including some stepped stepped surfaces.
- g. (110) terraces with (100) steps

[Note: the (310) face, although listed among (111) terrace surfaces, has (100) terraces and therefore (110) steps.]

TERRACE ORIENTATION (1 1 1)

MICROFACET EDGE VECTORS TO SERVE AS BASIS VECTORS (-.5 .5 0.) (0. -.5 -.5) (0. -.5 .5)

SURFACE	ALGEBRAIC AND UNIT CELL DECOMPOSITION ON MICROFACETS (1 1 1) (1 1 -1) (1 0 0)	STEP NORMAL	ATOM TYPES KINK/ OTHER STEP/ TERRACE/ ALL	TERR EDGE VECT E IN CART. COORD. IN BASIS VECT.S	TERR WIDTH VECT W IN CART. COORD. IN BASIS VECT.S	LENGTH OF E	LENGTH OF W	ANGLE BETWEEN E AND W	SPOT SPLIT- TING	SPOT ROW SPACING TO SPOT SPLITTING RATIO
(1 1 0)	.5 .5 0. 1UC 1UC 0UC	(1 1 -1)	0 1 1 2	(.50 -.50 0.) (-1.00 0. 0.)	(0. 0. 1.00) (0. -1.00 1.00)	.7071	1.0000	90.0000	1.0000	1.4142
(3 3 1)	2.0 1.0 0. 2UC 1UC 0UC	(1 1 -1)	0 1 2 3	(.50 -.50 0.) (-1.00 0. 0.)	(0. -.50 1.50) (0. -1.00 2.00)	.7071	1.5811	77.0790	.6489	2.1794
(2 2 1)	1.5 .5 0. 3UC 1UC 0UC	(1 1 -1)	0 1 3 4	(.50 -.50 0.) (-1.00 0. 0.)	(-.50 -.50 2.00) (1.00 -1.00 3.00)	.7071	2.1213	90.0000	.4714	3.0000
(5 5 3)	4.0 1.0 0. 4UC 1UC 0UC	(1 1 -1)	0 1 4 5	(.50 -.50 0.) (-1.00 0. 0.)	(-.50 -1.00 2.50) (1.00 -1.00 4.00)	.7071	2.7386	82.5824	.3682	3.8406
(3 3 2)	2.5 .5 0. 5UC 1UC 0UC	(1 1 -1)	0 1 5 6	(.50 -.50 0.) (-1.00 0. 0.)	(-1.00 -1.00 3.00) (2.00 -1.00 5.00)	.7071	3.3166	90.0000	.3015	4.6904
(7 7 5)	6.0 1.0 0. 6UC 1UC 0UC	(1 1 -1)	0 1 6 7	(.50 -.50 0.) (-1.00 0. 0.)	(-1.00 -1.50 3.50) (2.00 -1.00 6.00)	.7071	3.9370	84.8477	.2550	5.5453
(4 4 3)	3.5 .5 0. 7UC 1UC 0UC	(1 1 -1)	0 1 7 8	(.50 -.50 0.) (-1.00 0. 0.)	(-1.50 -1.50 4.00) (3.00 -1.00 7.00)	.7071	4.5277	90.0000	.2209	6.4031
(9 9 7)	8.0 1.0 0. 8UC 1UC 0UC	(1 1 -1)	0 1 8 9	(.50 -.50 0.) (-1.00 0. 0.)	(-1.50 -2.00 4.50) (3.00 -1.00 8.00)	.7071	5.1478	86.0618	.1947	7.2629
(5 5 4)	4.5 .5 0. 9UC 1UC 0UC	(1 1 -1)	0 1 9 10	(.50 -.50 0.) (-1.00 0. 0.)	(-2.00 -2.00 5.00) (4.00 -1.00 9.00)	.7071	5.7446	90.0000	.1741	8.1240
(1111 9)	10.0 1.0 0. 10UC 1UC 0UC	(1 1 -1)	0 1 10 11	(.50 -.50 0.) (-1.00 0. 0.)	(-2.00 -2.50 5.50) (4.00 -1.00 10.00)	.7071	6.3640	86.8153	.1574	8.9861
(6 6 5)	5.5 .5 0. 11UC 1UC 0UC	(1 1 -1)	0 1 11 12	(.50 -.50 0.) (-1.00 0. 0.)	(-2.50 -2.50 6.00) (5.00 -1.00 11.00)	.7071	6.9642	90.0000	.1436	9.8489
(131311)	12.0 1.0 0. 12UC 1UC 0UC	(1 1 -1)	0 1 12 13	(.50 -.50 0.) (-1.00 0. 0.)	(-2.50 -3.00 6.50) (5.00 -1.00 12.00)	.7071	7.5829	87.3276	.1320	10.7121
(7 7 6)	6.5 .5 0. 13UC 1UC 0UC	(1 1 -1)	0 1 13 14	(.50 -.50 0.) (-1.00 0. 0.)	(-3.00 -3.00 7.00) (6.00 -1.00 13.00)	.7071	8.1854	90.0000	.1222	11.5758
(151513)	14.0 1.0 0. 14UC 1UC 0UC	(1 1 -1)	0 1 14 15	(.50 -.50 0.) (-1.00 0. 0.)	(-3.00 -3.50 7.50) (6.00 -1.00 14.00)	.7071	8.8034	87.6983	.1137	12.4399
(8 8 7)	7.5 .5 0. 15UC 1UC 0UC	(1 1 -1)	0 1 15 16	(.50 -.50 0.) (-1.00 0. 0.)	(-3.50 -3.50 8.00) (7.00 -1.00 15.00)	.7071	9.4074	90.0000	.1063	13.3041
(171715)	16.0 1.0 0. 16UC 1UC 0UC	(1 1 -1)	0 1 16 17	(.50 -.50 0.) (-1.00 0. 0.)	(-3.50 -4.00 8.50) (7.00 -1.00 16.00)	.7071	10.0250	87.9789	.0998	14.1686
(9 9 8)	8.5 .5 0. 17UC 1UC 0UC	(1 1 -1)	0 1 17 18	(.50 -.50 0.) (-1.00 0. 0.)	(-4.00 -4.00 9.00) (8.00 -1.00 17.00)	.7071	10.6301	90.0000	.0941	15.0333
(191917)	18.0 1.0 0. 18UC 1UC 0UC	(1 1 -1)	0 1 18 19	(.50 -.50 0.) (-1.00 0. 0.)	(-4.00 -4.50 9.50) (8.00 -1.00 18.00)	.7071	11.2472	88.1986	.0890	15.8981
(1010 9)	9.5 .5 0. 19UC 1UC 0UC	(1 1 -1)	0 1 19 20	(.50 -.50 0.) (-1.00 0. 0.)	(-4.50 -4.50 10.00) (9.00 -1.00 19.00)	.7071	11.8533	90.0000	.0844	16.7631

TERRACE ORIENTATION (1 1 1)

MICROFACET EDGE VECTORS TO SERVE AS BASIS VECTORS (-.5 .5 0.) (0. -.5 .5) (0. -.5 .5)

SURFACE	ALGEBRAIC AND UNIT CELL DECOMPOSITION ON MICROFACETS (1 1 1) (1 1 -1) (1 0 0)	STEP NORMAL	ATOM TYPES KINK/ OTHER STEP/ TERRACE/ ALL	TERR EDGE VECT E IN CART. COORD. IN BASIS VECT.S	TERR WIDTH VECT W IN CART. COORD. IN BASIS VECT.S	LENGTH OF E	LENGTH OF W	ANGLE BETWEEN E AND W	SPOT SPLIT- TING	SPOT ROW SPACING TO SPOT SPLITTING RATIO
(3 1 1)	1.0 0. 2.0 (1 0 0) 1UC OUC 1UC	(1 0 0)	0 1 1 2	(0. -.50 .50) (0. 0. 1.00)	(-.50 .50 1.00) (1.00-1.00 1.00)	.7071	1.2247	73.2213	.8528	1.6583
(2 1 1)	1.0 0. 1.0 (1 0 0) 2UC OUC 1UC	(1 0 0)	0 1 2 3	(0. -.50 .50) (0. 0. 1.00)	(-1.00 1.00 1.00) (2.00-1.00 1.00)	.7071	1.7321	90.0000	.5774	2.4495
(5 3 3)	3.0 0. 2.0 (1 0 0) 3UC OUC 1UC	(1 0 0)	0 1 3 4	(0. -.50 .50) (0. 0. 1.00)	(-1.50 1.00 1.50) (3.00-1.00 2.00)	.7071	2.3452	81.3293	.4313	3.2787
(3 2 2)	2.0 0. 1.0 (1 0 0) 4UC OUC 1UC	(1 0 0)	0 1 4 5	(0. -.50 .50) (0. 0. 1.00)	(-2.00 1.50 1.50) (4.00-1.00 2.00)	.7071	2.9155	90.0000	.3430	4.1231
(7 5 5)	5.0 0. 2.0 (1 0 0) 5UC OUC 1UC	(1 0 0)	0 1 5 6	(0. -.50 .50) (0. 0. 1.00)	(-2.50 1.50 2.00) (5.00-1.00 3.00)	.7071	3.5355	84.2608	.2843	4.9749
(4 3 3)	3.0 0. 1.0 (1 0 0) 6UC OUC 1UC	(1 0 0)	0 1 6 7	(0. -.50 .50) (0. 0. 1.00)	(-3.00 2.00 2.00) (6.00-1.00 3.00)	.7071	4.1231	90.0000	.2425	5.8310
(9 7 7)	7.0 0. 2.0 (1 0 0) 7UC OUC 1UC	(1 0 0)	0 1 7 8	(0. -.50 .50) (0. 0. 1.00)	(-3.50 2.00 2.50) (7.00-1.00 4.00)	.7071	4.7434	85.7255	.2114	6.6895
(5 4 4)	4.0 0. 1.0 (1 0 0) 8UC OUC 1UC	(1 0 0)	0 1 8 9	(0. -.50 .50) (0. 0. 1.00)	(-4.00 2.50 2.50) (8.00-1.00 4.00)	.7071	5.3385	90.0000	.1873	7.5498
(11 9 9)	9.0 0. 2.0 (1 0 0) 9UC OUC 1UC	(1 0 0)	0 1 9 10	(0. -.50 .50) (0. 0. 1.00)	(-4.50 2.50 3.00) (9.00-1.00 5.00)	.7071	5.9582	86.5981	.1681	8.4113
(6 5 5)	5.0 0. 1.0 (1 0 0) 10UC OUC 1UC	(1 0 0)	0 1 10 11	(0. -.50 .50) (0. 0. 1.00)	(-5.00 3.00 3.00) (10.00-1.00 5.00)	.7071	6.5574	90.0000	.1525	9.2736
(13 11 11)	11.0 0. 2.0 (1 0 0) 11UC OUC 1UC	(1 0 0)	0 1 11 12	(0. -.50 .50) (0. 0. 1.00)	(-5.50 3.00 3.50) (11.00-1.00 6.00)	.7071	7.1764	87.1761	.1395	10.1366
(7 6 6)	6.0 0. 1.0 (1 0 0) 12UC OUC 1UC	(1 0 0)	0 1 12 13	(0. -.50 .50) (0. 0. 1.00)	(-6.00 3.50 3.50) (12.00-1.00 6.00)	.7071	7.7782	90.0000	.1286	11.0000
(15 13 13)	13.0 0. 2.0 (1 0 0) 13UC OUC 1UC	(1 0 0)	0 1 13 14	(0. -.50 .50) (0. 0. 1.00)	(-6.50 3.50 4.00) (13.00-1.00 7.00)	.7071	8.3964	87.5867	.1192	11.8638
(8 7 7)	7.0 0. 1.0 (1 0 0) 14UC OUC 1UC	(1 0 0)	0 1 14 15	(0. -.50 .50) (0. 0. 1.00)	(-7.00 4.00 4.00) (14.00-1.00 7.00)	.7071	9.0000	90.0000	.1111	12.7279
(17 15 15)	15.0 0. 2.0 (1 0 0) 15UC OUC 1UC	(1 0 0)	0 1 15 16	(0. -.50 .50) (0. 0. 1.00)	(-7.50 4.00 4.50) (15.00-1.00 8.00)	.7071	9.6177	87.8933	.1040	13.5923
(9 8 8)	8.0 0. 1.0 (1 0 0) 16UC OUC 1UC	(1 0 0)	0 1 16 17	(0. -.50 .50) (0. 0. 1.00)	(-8.00 4.50 4.50) (16.00-1.00 8.00)	.7071	10.2225	90.0000	.0978	14.4568
(19 17 17)	17.0 0. 2.0 (1 0 0) 17UC OUC 1UC	(1 0 0)	0 1 17 18	(0. -.50 .50) (0. 0. 1.00)	(-8.50 4.50 5.00) (17.00-1.00 9.00)	.7071	10.8397	88.1309	.0923	15.3216
(10 9 9)	9.0 0. 1.0 (1 0 0) 18UC OUC 1UC	(1 0 0)	0 1 18 19	(0. -.50 .50) (0. 0. 1.00)	(-9.00 5.00 5.00) (18.00-1.00 9.00)	.7071	11.4455	90.0000	.0874	16.1864
(21 19 19)	19.0 0. 2.0 (1 0 0) 19UC OUC 1UC	(1 0 0)	0 1 19 20	(0. -.50 .50) (0. 0. 1.00)	(-9.50 5.00 5.50) (19.00-1.00 10.00)	.7071	12.0623	88.3204	.0829	17.0514

TERRACE ORIENTATION (1 1 1)

MICROFACET EDGE VECTORS TO SERVE AS BASIS VECTORS (-.5 .5 0.) (0. -.5 -.5) (0. -.5 .5)

SURFACE	ALGEBRAIC AND UNIT CELL DECOMPOSITION ON MICROFACETS (1 1 1) (1 1 -1) (1 0 0)	STEP NORMAL	ATOM TYPES KINK/ OTHER STEP/ TERRACE/ ALL	TERR EDGE VECT E IN CART. COORD. IN BASIS VECT.S	TERR WIDTH VECT W IN CART. COORD. IN BASIS VECT.S	LENGTH OF E	LENGTH OF W	ANGLE BETWEEN E AND W	SPOT SPLIT- TING	SPOT ROW SPACING TO SPOT SPLITTING RATIO
(3 1 0)	.5 .5 2.0 (1 1 0) 1UC 1UC 2UC	(1 1 0)	1 1 2 4	(0. 0. -1.00) (.50-1.50 0.) (0. 1.00-1.00) (-1.00 1.00 1.00)	(.50-1.50 0.) (-1.00 1.00 1.00)	1.0000	1.5811	90.0000	.6325	1.5811
(4 2 1)	1.5 .5 2.0 (5 1 -1) 3UC 1UC 2UC	(5 1 -1)	1 2 3 6	(.50-1.50 1.00) (-.50 .50 1.00) (-1.00 0. 2.00) (1.00-1.00 1.00)	(-.50 .50 1.00) (1.00-1.00 1.00)	1.8708	1.2247	90.0000	.8165	.6547
(5 3 2)	2.5 .5 2.0 (5 1 -1) 5UC 1UC 2UC	(5 1 -1)	1 2 5 8	(.50-1.50 1.00) (-1.00 1.00 1.00) (-1.00 0. 2.00) (2.00-1.00 1.00)	(-1.00 1.00 1.00) (2.00-1.00 1.00)	1.8708	1.7321	107.9753	.6070	.8806
(6 4 3)	3.5 .5 2.0 (5 1 -1) 7UC 1UC 2UC	(5 1 -1)	1 2 7 10	(.50-1.50 1.00) (-1.00 -.00 2.00) (-1.00 0. 2.00) (2.00-1.00 3.00)	(-1.00 -.00 2.00) (2.00-1.00 3.00)	1.8708	2.2361	68.9877	.4791	1.1157
(7 5 4)	4.5 .5 2.0 (5 1 -1) 9UC 1UC 2UC	(5 1 -1)	1 2 9 12	(.50-1.50 1.00) (-1.50 .50 2.00) (-1.00 0. 2.00) (3.00-1.00 3.00)	(-1.50 .50 2.00) (3.00-1.00 3.00)	1.8708	2.5495	83.9827	.3944	1.3553
(8 6 5)	5.5 .5 2.0 (5 1 -1) 11UC 1UC 2UC	(5 1 -1)	1 2 11 14	(.50-1.50 1.00) (-2.00 1.00 2.00) (-1.00 0. 2.00) (4.00-1.00 3.00)	(-2.00 1.00 2.00) (4.00-1.00 3.00)	1.8708	3.0000	95.1111	.3347	1.5972
(9 7 6)	6.5 .5 2.0 (5 1 -1) 13UC 1UC 2UC	(5 1 -1)	1 2 13 16	(.50-1.50 1.00) (-2.50 1.50 2.00) (-1.00 0. 2.00) (5.00-1.00 3.00)	(-2.50 1.50 2.00) (5.00-1.00 3.00)	1.8708	3.5355	103.1075	.2904	1.8406
(10 8 7)	7.5 .5 2.0 (5 1 -1) 15UC 1UC 2UC	(5 1 -1)	1 2 15 18	(.50-1.50 1.00) (-2.50 .50 3.00) (-1.00 0. 2.00) (5.00-1.00 5.00)	(-2.50 .50 3.00) (5.00-1.00 5.00)	1.8708	3.9370	82.1969	.2564	2.0849
(11 9 8)	8.5 .5 2.0 (5 1 -1) 17UC 1UC 2UC	(5 1 -1)	1 2 17 20	(.50-1.50 1.00) (-3.00 1.00 3.00) (-1.00 0. 2.00) (6.00-1.00 5.00)	(-3.00 1.00 3.00) (6.00-1.00 5.00)	1.8708	4.3589	90.0000	.2294	2.3299
(12 10 9)	9.5 .5 2.0 (5 1 -1) 19UC 1UC 2UC	(5 1 -1)	1 2 19 22	(.50-1.50 1.00) (-3.50 1.50 3.00) (-1.00 0. 2.00) (7.00-1.00 5.00)	(-3.50 1.50 3.00) (7.00-1.00 5.00)	1.8708	4.8477	96.3305	.2075	2.5754
(13 11 10)	10.5 .5 2.0 (5 1 -1) 21UC 1UC 2UC	(5 1 -1)	1 2 21 24	(.50-1.50 1.00) (-3.50 .50 4.00) (-1.00 0. 2.00) (7.00-1.00 7.00)	(-3.50 .50 4.00) (7.00-1.00 7.00)	1.8708	5.3385	81.3622	.1895	2.8212
(14 12 11)	11.5 .5 2.0 (5 1 -1) 23UC 1UC 2UC	(5 1 -1)	1 2 23 26	(.50-1.50 1.00) (-4.00 1.00 4.00) (-1.00 0. 2.00) (8.00-1.00 7.00)	(-4.00 1.00 4.00) (8.00-1.00 7.00)	1.8708	5.7446	87.3334	.1743	3.0673
(15 13 12)	12.5 .5 2.0 (5 1 -1) 25UC 1UC 2UC	(5 1 -1)	1 2 25 28	(.50-1.50 1.00) (-4.50 1.50 4.00) (-1.00 0. 2.00) (9.00-1.00 7.00)	(-4.50 1.50 4.00) (9.00-1.00 7.00)	1.8708	6.2048	92.4687	.1613	3.3135
(16 14 13)	13.5 .5 2.0 (5 1 -1) 27UC 1UC 2UC	(5 1 -1)	1 2 27 30	(.50-1.50 1.00) (-5.00 2.00 4.00) (-1.00 0. 2.00) (10.00-1.00 7.00)	(-5.00 2.00 4.00) (10.00-1.00 7.00)	1.8708	6.7082	96.8646	.1501	3.5600
(17 15 14)	14.5 .5 2.0 (5 1 -1) 29UC 1UC 2UC	(5 1 -1)	1 2 29 32	(.50-1.50 1.00) (-5.00 1.00 5.00) (-1.00 0. 2.00) (10.00-1.00 9.00)	(-5.00 1.00 5.00) (10.00-1.00 9.00)	1.8708	7.1414	85.7075	.1404	3.8065
(18 16 15)	15.5 .5 2.0 (5 1 -1) 31UC 1UC 2UC	(5 1 -1)	1 2 31 34	(.50-1.50 1.00) (-5.50 1.50 5.00) (-1.00 0. 2.00) (11.00-1.00 9.00)	(-5.50 1.50 5.00) (11.00-1.00 9.00)	1.8708	7.5829	90.0000	.1319	4.0532
(19 17 16)	16.5 .5 2.0 (5 1 -1) 33UC 1UC 2UC	(5 1 -1)	1 2 33 36	(.50-1.50 1.00) (-6.00 2.00 5.00) (-1.00 0. 2.00) (12.00-1.00 9.00)	(-6.00 2.00 5.00) (12.00-1.00 9.00)	1.8708	8.0623	93.8015	.1243	4.3000
(20 18 17)	17.5 .5 2.0 (5 1 -1) 35UC 1UC 2UC	(5 1 -1)	1 2 35 38	(.50-1.50 1.00) (-6.00 1.00 6.00) (-1.00 0. 2.00) (12.00-1.00 11.00)	(-6.00 1.00 6.00) (12.00-1.00 11.00)	1.8708	8.5440	84.6153	.1176	4.5468
(21 19 18)	18.5 .5 2.0 (5 1 -1) 37UC 1UC 2UC	(5 1 -1)	1 2 37 40	(.50-1.50 1.00) (-6.50 1.50 6.00) (-1.00 0. 2.00) (13.00-1.00 11.00)	(-6.50 1.50 6.00) (13.00-1.00 11.00)	1.8708	8.9722	88.2930	.1115	4.7937
(22 20 19)	19.5 .5 2.0 (5 1 -1) 39UC 1UC 2UC	(5 1 -1)	1 2 39 42	(.50-1.50 1.00) (-7.00 2.00 6.00) (-1.00 0. 2.00) (14.00-1.00 11.00)	(-7.00 2.00 6.00) (14.00-1.00 11.00)	1.8708	9.4340	91.6234	.1060	5.0407

Table 2c

TERRACE ORIENTATION (1 0 0)

MICROFACET EDGE VECTORS TO SERVE AS BASIS VECTORS (-.5 .5 0.) (0. -.5 -.5) (0. -.5 .5)

SURFACE	ALGEBRAIC AND UNIT CELL DECOMPOSITION ON MICROFACETS (1 1 1) (1 1 -1) (1 0 0)	STEP NORMAL	ATOM TYPES KINK/ OTHER STEP/ TERRACE/ ALL	TERR EDGE VECT E IN CART. COORD. IN BASIS VECT.S	TERR WIDTH VECT W IN CART. COORD. IN BASIS VECT.S	LENGTH OF E	LENGTH OF W	ANGLE BETWEEN E AND W	SPOT SPLIT- TING	SPOT ROW SPACING TO SPOT SPLITTING RATIO
(2 1-1)	0. 1.0 1.0 (1 0 0) OUC 2UC 1UC	(1 0 0)	0 1 2 3	(0. .50 .50) (0. -1.00 0.)	(-1.00 1.00 -1.00) (2.00 1.00 -1.00)	.7071	1.7321	90.0000	.5774	2.4495
(3 1-1)	0. 1.0 2.0 (1 1-1) OUC 1UC 1UC	(1 1-1)	0 1 1 2	(0. .50 .50) (0. -1.00 0.)	(-.50 1.00 -.50) (1.00 0. -1.00)	.7071	1.2247	73.2213	.8528	1.6583
(4 1-1)	0. 1.0 3.0 (1 1-1) OUC 2UC 3UC	(1 1-1)	0 2 3 5	(0. .50 -.50) (0. 1.00 0.)	(1.00-2.00 2.00) (-2.00-1.00 3.00)	.7071	3.0000	90.0000	.3333	4.2426
(5 1-1)	0. 1.0 4.0 (1 1-1) OUC 1UC 2UC	(1 1-1)	0 1 2 3	(0. -.50 -.50) (0. 1.00 0.)	(.50-1.50 1.00) (-1.00 0. 2.00)	.7071	1.8708	79.1066	.5443	2.5981
(6 1-1)	0. 1.0 5.0 (1 1-1) OUC 2UC 5UC	(1 1-1)	0 2 5 7	(0. -.50 -.50) (0. 1.00 0.)	(1.00-3.00 3.00) (-2.00-1.00 5.00)	.7071	4.3589	90.0000	.2294	6.1644
(7 1-1)	0. 1.0 6.0 (1 1-1) OUC 1UC 3UC	(1 1-1)	0 1 3 4	(0. -.50 -.50) (0. 1.00 0.)	(.50-2.00 1.50) (-1.00 0. 3.00)	.7071	2.5495	82.0288	.3961	3.5707
(8 1-1)	0. 1.0 7.0 (1 1-1) OUC 2UC 7UC	(1 1-1)	0 2 7 9	(0. -.50 -.50) (0. 1.00 0.)	(1.00-4.00 4.00) (-2.00-1.00 7.00)	.7071	5.7446	90.0000	.1741	8.1240
(9 1-1)	0. 1.0 8.0 (1 1-1) OUC 1UC 4UC	(1 1-1)	0 1 4 5	(0. -.50 -.50) (0. 1.00 0.)	(.50-2.50 2.00) (-1.00 0. 4.00)	.7071	3.2404	83.7360	.3105	4.5552
(10 1-1)	0. 1.0 9.0 (1 1-1) OUC 2UC 9UC	(1 1-1)	0 2 9 11	(0. -.50 -.50) (0. 1.00 0.)	(1.00-5.00 5.00) (-2.00-1.00 9.00)	.7071	7.1414	90.0000	.1400	10.0995
(11 1-1)	0. 1.010.0 (1 1-1) OUC 1UC 5UC	(1 1-1)	0 1 5 6	(0. -.50 -.50) (0. 1.00 0.)	(.50-3.00 2.50) (-1.00 0. 5.00)	.7071	3.9370	84.8477	.2550	5.5453
(12 1-1)	0. 1.011.0 (1 1-1) OUC 2UC11UC	(1 1-1)	0 2 11 13	(0. -.50 -.50) (0. 1.00 0.)	(1.00-6.00 6.00) (-2.00-1.0011.00)	.7071	8.5440	90.0000	.1170	12.0830
(13 1-1)	0. 1.012.0 (1 1-1) OUC 1UC 6UC	(1 1-1)	0 1 6 7	(0. -.50 -.50) (0. 1.00 0.)	(.50-3.50 3.00) (-1.00 0. 6.00)	.7071	4.6368	85.6270	.2163	6.5383
(14 1-1)	0. 1.013.0 (1 1-1) OUC 2UC13UC	(1 1-1)	0 2 13 15	(0. -.50 -.50) (0. 1.00 0.)	(1.00-7.00 7.00) (-2.00-1.0013.00)	.7071	9.9499	90.0000	.1005	14.0712
(15 1-1)	0. 1.014.0 (1 1-1) OUC 1UC 7UC	(1 1-1)	0 1 7 8	(0. -.50 -.50) (0. 1.00 0.)	(.50-4.00 3.50) (-1.00 0. 7.00)	.7071	5.3385	86.2027	.1877	7.5333
(16 1-1)	0. 1.015.0 (1 1-1) OUC 2UC15UC	(1 1-1)	0 2 15 17	(0. -.50 -.50) (0. 1.00 0.)	(1.00-8.00 8.00) (-2.00-1.0015.00)	.7071	11.3578	90.0000	.0880	16.0624
(17 1-1)	0. 1.016.0 (1 1-1) OUC 1UC 8UC	(1 1-1)	0 1 8 9	(0. -.50 -.50) (0. 1.00 0.)	(.50-4.50 4.00) (-1.00 0. 8.00)	.7071	6.0415	86.6451	.1658	8.5294
(18 1-1)	0. 1.017.0 (1 1-1) OUC 2UC17UC	(1 1-1)	0 2 17 19	(0. -.50 -.50) (0. 1.00 0.)	(1.00-9.00 9.00) (-2.00-1.0017.00)	.7071	12.7671	90.0000	.0783	18.0555
(19 1-1)	0. 1.018.0 (1 1-1) OUC 1UC 9UC	(1 1-1)	0 1 9 10	(0. -.50 -.50) (0. 1.00 0.)	(.50-5.00 4.50) (-1.00 0. 9.00)	.7071	6.7454	86.9955	.1485	9.5263
(20 1-1)	0. 1.019.0 (1 1-1) OUC 2UC19UC	(1 1-1)	0 2 19 21	(0. -.50 -.50) (0. 1.00 0.)	(1.00-10.010.00) (-2.00-1.0019.00)	.7071	14.1774	90.0000	.0705	20.0499

Table 2d

TERRACE ORIENTATION (1 0 0)

MICROFACET EDGE VECTORS TO SERVE AS BASIS VECTORS (-.5 .5 0.) (0. 0. -1.0) (0. -.5 .5)

SURFACE	ALGEBRAIC AND UNIT CELL DECOMPOSITION ON MICROFACETS (1 1 1) (1 1 0) (1 0 0)	STEP NORMAL	ATOM TYPES KINK/ OTHER STEP/ TERRACE/ ALL	TERR EDGE VECT E IN CART. COORD. IN BASIS VECT.S	TERR WIDTH VECT W IN CART. COORD. IN BASIS VECT.S	LENGTH OF E	LENGTH OF W	ANGLE BETWEEN E AND W	SPOT SPLIT- TING	SPOT ROW SPACING TO SPOT SPLITTING RATIO
(2 1 0)	0. 1.0 1.0 (1 1 0) OUC 1UC 1UC	(1 1 0)	0 1 1 2	(0. 0. 1.00) (-.50 1.00 .50) (0. -1.00 0.) (1.00 -1.00 -1.00)	(-.50 1.00 .50) (1.00 -1.00 -1.00)	1.0000	1.2247	65.9052	.8944	1.1180
(3 1 0)	0. 1.0 2.0 (1 1 0) OUC 1UC 2UC	(1 1 0)	0 1 2 3	(0. 0. -1.00) (.50 -1.50 0.) (0. 1.00 0.) (-1.00 1.00 2.00)	(.50 -1.50 0.) (-1.00 1.00 2.00)	1.0000	1.5811	90.0000	.6325	1.5811
(4 1 0)	0. 1.0 3.0 (1 1 0) OUC 1UC 3UC	(1 1 0)	0 1 3 4	(0. 0. -1.00) (.50 -2.00 -.50) (0. 1.00 0.) (-1.00 2.00 3.00)	(.50 -2.00 -.50) (-1.00 2.00 3.00)	1.0000	2.1213	76.3670	.4851	2.0616
(5 1 0)	0. 1.0 4.0 (1 1 0) OUC 1UC 4UC	(1 1 0)	0 1 4 5	(0. 0. -1.00) (.50 -2.50 0.) (0. 1.00 0.) (-1.00 2.00 4.00)	(.50 -2.50 0.) (-1.00 2.00 4.00)	1.0000	2.5495	90.0000	.3922	2.5495
(6 1 0)	0. 1.0 5.0 (1 1 0) OUC 1UC 5UC	(1 1 0)	0 1 5 6	(0. 0. -1.00) (.50 -3.00 -.50) (0. 1.00 0.) (-1.00 3.00 5.00)	(.50 -3.00 -.50) (-1.00 3.00 5.00)	1.0000	3.0822	80.6641	.3288	3.0414
(7 1 0)	0. 1.0 6.0 (1 1 0) OUC 1UC 6UC	(1 1 0)	0 1 6 7	(0. 0. -1.00) (.50 -3.50 0.) (0. 1.00 0.) (-1.00 3.00 6.00)	(.50 -3.50 0.) (-1.00 3.00 6.00)	1.0000	3.5355	90.0000	.2828	3.5355
(8 1 0)	0. 1.0 7.0 (1 1 0) OUC 1UC 7UC	(1 1 0)	0 1 7 8	(0. 0. -1.00) (.50 -4.00 -.50) (0. 1.00 0.) (-1.00 4.00 7.00)	(.50 -4.00 -.50) (-1.00 4.00 7.00)	1.0000	4.0620	82.9294	.2481	4.0311
(9 1 0)	0. 1.0 8.0 (1 1 0) OUC 1UC 8UC	(1 1 0)	0 1 8 9	(0. 0. -1.00) (.50 -4.50 0.) (0. 1.00 0.) (-1.00 4.00 8.00)	(.50 -4.50 0.) (-1.00 4.00 8.00)	1.0000	4.5277	90.0000	.2209	4.5277
(10 1 0)	0. 1.0 9.0 (1 1 0) OUC 1UC 9UC	(1 1 0)	0 1 9 10	(0. 0. -1.00) (.50 -5.00 -.50) (0. 1.00 0.) (-1.00 5.00 9.00)	(.50 -5.00 -.50) (-1.00 5.00 9.00)	1.0000	5.0498	84.3176	.1990	5.0249
(11 1 0)	0. 1.0 10.0 (1 1 0) OUC 1UC 10UC	(1 1 0)	0 1 10 11	(0. 0. -1.00) (.50 -5.50 0.) (0. 1.00 0.) (-1.00 5.00 10.00)	(.50 -5.50 0.) (-1.00 5.00 10.00)	1.0000	5.5227	90.0000	.1811	5.5227
(12 1 0)	0. 1.0 11.0 (1 1 0) OUC 1UC 11UC	(1 1 0)	0 1 11 12	(0. 0. -1.00) (.50 -6.00 -.50) (0. 1.00 0.) (-1.00 6.00 11.00)	(.50 -6.00 -.50) (-1.00 6.00 11.00)	1.0000	6.0415	85.2527	.1661	6.0208
(13 1 0)	0. 1.0 12.0 (1 1 0) OUC 1UC 12UC	(1 1 0)	0 1 12 13	(0. 0. -1.00) (.50 -6.50 0.) (0. 1.00 0.) (-1.00 6.00 12.00)	(.50 -6.50 0.) (-1.00 6.00 12.00)	1.0000	6.5192	90.0000	.1534	6.5192
(14 1 0)	0. 1.0 13.0 (1 1 0) OUC 1UC 13UC	(1 1 0)	0 1 13 14	(0. 0. -1.00) (.50 -7.00 -.50) (0. 1.00 0.) (-1.00 7.00 13.00)	(.50 -7.00 -.50) (-1.00 7.00 13.00)	1.0000	7.0356	85.9247	.1425	7.0178
(15 1 0)	0. 1.0 14.0 (1 1 0) OUC 1UC 14UC	(1 1 0)	0 1 14 15	(0. 0. -1.00) (.50 -7.50 0.) (0. 1.00 0.) (-1.00 7.00 14.00)	(.50 -7.50 0.) (-1.00 7.00 14.00)	1.0000	7.5166	90.0000	.1330	7.5166
(16 1 0)	0. 1.0 15.0 (1 1 0) OUC 1UC 15UC	(1 1 0)	0 1 15 16	(0. 0. -1.00) (.50 -8.00 -.50) (0. 1.00 0.) (-1.00 8.00 15.00)	(.50 -8.00 -.50) (-1.00 8.00 15.00)	1.0000	8.0312	86.4306	.1248	8.0156
(17 1 0)	0. 1.0 16.0 (1 1 0) OUC 1UC 16UC	(1 1 0)	0 1 16 17	(0. 0. -1.00) (.50 -8.50 0.) (0. 1.00 0.) (-1.00 8.00 16.00)	(.50 -8.50 0.) (-1.00 8.00 16.00)	1.0000	8.5147	90.0000	.1174	8.5147
(18 1 0)	0. 1.0 17.0 (1 1 0) OUC 1UC 17UC	(1 1 0)	0 1 17 18	(0. 0. -1.00) (.50 -9.00 -.50) (0. 1.00 0.) (-1.00 9.00 17.00)	(.50 -9.00 -.50) (-1.00 9.00 17.00)	1.0000	9.0277	86.8251	.1109	9.0139
(19 1 0)	0. 1.0 18.0 (1 1 0) OUC 1UC 18UC	(1 1 0)	0 1 18 19	(0. 0. -1.00) (.50 -9.50 0.) (0. 1.00 0.) (-1.00 9.00 18.00)	(.50 -9.50 0.) (-1.00 9.00 18.00)	1.0000	9.5131	90.0000	.1051	9.5131
(20 1 0)	0. 1.0 19.0 (1 1 0) OUC 1UC 19UC	(1 1 0)	0 1 19 20	(0. 0. -1.00) (.50 -10.0 -.50) (0. 1.00 0.) (-1.00 10.00 19.00)	(.50 -10.0 -.50) (-1.00 10.00 19.00)	1.0000	10.0250	87.1412	.0999	10.0125

Table 2c

TERRACE ORIENTATION (1 1 0)

MICROFACET EDGE VECTORS TO SERVE AS BASIS VECTORS (-.5 .5 0.) (0. 0. -1.0) (0. -.5 .5)

SURFACE	ALGEBRAIC AND UNIT CELL DECOMPOSITION ON MICROFACETS (1 1 1) (1 1 0) (1 0 0)	STEP NORMAL	ATOM TYPES KINK/ OTHER STEP/ TERRACE/ ALL	TERR EDGE VECT E IN CART. COORD. IN BASIS VECT.S	TERR WIDTH VECT W IN CART. COORD. IN BASIS VECT.S	LENGTH OF E	LENGTH OF W	ANGLE BETWEEN E AND W	SPOT SPLIT- TING	SPOT ROW SPACING TO SPOT SPLITTING RATIO
(2 2 1)	1.0 1.0 0. (1 1 0) 2UC 1UC OUC	(1 1 0)	0 1 2 3	(-.50 -.50 0.) (-.50 -.50 2.00) (-1.00 0. 0.) (1.00 -1.00 2.00)	(-.50 -.50 2.00) (1.00 -1.00 2.00)	.7071	2.1213	90.0000	.4714	3.0000
(3 3 1)	1.0 2.0 0. (1 1 1) 1UC 1UC OUC	(1 1 1)	0 1 1 2	(-.50 -.50 0.) (0. -.50 1.50) (-1.00 0. 0.) (0. -1.00 1.00)	(0. -.50 1.50) (0. -1.00 1.00)	.7071	1.5811	77.0790	.6489	2.1794
(4 4 1)	1.0 3.0 0. (1 1 1) 2UC 3UC OUC	(1 1 1)	0 2 3 5	(-.50 .50 0.) (.50 .50 -4.00) (1.00 0. 0.) (-1.00 3.00 -2.00)	(.50 .50 -4.00) (-1.00 3.00 -2.00)	.7071	4.0620	90.0000	.2462	5.7446
(5 5 1)	1.0 4.0 0. (1 1 1) 1UC 2UC OUC	(1 1 1)	0 1 2 3	(-.50 .50 0.) (0. .50 -2.50) (1.00 0. 0.) (0. 2.00 -1.00)	(0. .50 -2.50) (0. 2.00 -1.00)	.7071	2.5495	82.0288	.3961	3.5707
(6 6 1)	1.0 5.0 0. (1 1 1) 2UC 5UC OUC	(1 1 1)	0 2 5 7	(-.50 .50 0.) (.50 .50 -6.00) (1.00 0. 0.) (-1.00 5.00 -2.00)	(.50 .50 -6.00) (-1.00 5.00 -2.00)	.7071	6.0415	90.0000	.1655	8.5440
(7 7 1)	1.0 6.0 0. (1 1 1) 1UC 3UC OUC	(1 1 1)	0 1 3 4	(-.50 .50 0.) (0. .50 -3.50) (1.00 0. 0.) (0. 3.00 -1.00)	(0. .50 -3.50) (0. 3.00 -1.00)	.7071	3.5355	84.2608	.2843	4.9749
(8 8 1)	1.0 7.0 0. (1 1 1) 2UC 7UC OUC	(1 1 1)	0 2 7 9	(-.50 .50 0.) (.50 .50 -8.00) (1.00 0. 0.) (-1.00 7.00 -2.00)	(.50 .50 -8.00) (-1.00 7.00 -2.00)	.7071	8.0312	90.0000	.1245	11.3578
(9 9 1)	1.0 8.0 0. (1 1 1) 1UC 4UC OUC	(1 1 1)	0 1 4 5	(-.50 .50 0.) (0. .50 -4.50) (1.00 0. 0.) (0. 4.00 -1.00)	(0. .50 -4.50) (0. 4.00 -1.00)	.7071	4.5277	85.5214	.2215	6.3836
(1010 1)	1.0 9.0 0. (1 1 1) 2UC 9UC OUC	(1 1 1)	0 2 9 11	(-.50 .50 0.) (.50 .50 -10.0) (1.00 0. 0.) (-1.00 9.00 -2.00)	(.50 .50 -10.0) (-1.00 9.00 -2.00)	.7071	10.0250	90.0000	.0998	14.1774
(1111 1)	1.010.0 0. (1 1 1) 1UC 5UC OUC	(1 1 1)	0 1 5 6	(-.50 .50 0.) (0. .50 -5.50) (1.00 0. 0.) (0. 5.00 -1.00)	(0. .50 -5.50) (0. 5.00 -1.00)	.7071	5.5227	86.3295	.1814	7.7942
(1212 1)	1.011.0 0. (1 1 1) 2UC11UC OUC	(1 1 1)	0 2 11 13	(-.50 .50 0.) (.50 .50 -12.0) (1.00 0. 0.) (-1.0011.00 -2.00)	(.50 .50 -12.0) (-1.0011.00 -2.00)	.7071	12.0208	90.0000	.0832	17.0000
(1313 1)	1.012.0 0. (1 1 1) 1UC 6UC OUC	(1 1 1)	0 1 6 7	(-.50 .50 0.) (0. .50 -6.50) (1.00 0. 0.) (0. 6.00 -1.00)	(0. .50 -6.50) (0. 6.00 -1.00)	.7071	6.5192	86.8912	.1536	9.2060
(1414 1)	1.013.0 0. (1 1 1) 2UC13UC OUC	(1 1 1)	0 2 13 15	(-.50 .50 0.) (.50 .50 -14.0) (1.00 0. 0.) (-1.0013.00 -2.00)	(.50 .50 -14.0) (-1.0013.00 -2.00)	.7071	14.0178	90.0000	.0713	19.8242
(1515 1)	1.014.0 0. (1 1 1) 1UC 7UC OUC	(1 1 1)	0 1 7 8	(-.50 .50 0.) (0. .50 -7.50) (1.00 0. 0.) (0. 7.00 -1.00)	(0. .50 -7.50) (0. 7.00 -1.00)	.7071	7.5166	87.3040	.1332	10.6184
(1616 1)	1.015.0 0. (1 1 1) 2UC15UC OUC	(1 1 1)	0 2 15 17	(-.50 .50 0.) (.50 .50 -16.0) (1.00 0. 0.) (-1.0015.00 -2.00)	(.50 .50 -16.0) (-1.0015.00 -2.00)	.7071	16.0156	90.0000	.0624	22.6495
(1717 1)	1.016.0 0. (1 1 1) 1UC 8UC OUC	(1 1 1)	0 1 8 9	(-.50 .50 0.) (0. .50 -8.50) (1.00 0. 0.) (0. 8.00 -1.00)	(0. .50 -8.50) (0. 8.00 -1.00)	.7071	8.5147	87.6202	.1175	12.0312
(1818 1)	1.017.0 0. (1 1 1) 2UC17UC OUC	(1 1 1)	0 2 17 19	(-.50 .50 0.) (.50 .50 -18.0) (1.00 0. 0.) (-1.0017.00 -2.00)	(.50 .50 -18.0) (-1.0017.00 -2.00)	.7071	18.0139	90.0000	.0555	25.4755
(1919 1)	1.018.0 0. (1 1 1) 1UC 9UC OUC	(1 1 1)	0 1 9 10	(-.50 .50 0.) (0. .50 -9.50) (1.00 0. 0.) (0. 9.00 -1.00)	(0. .50 -9.50) (0. 9.00 -1.00)	.7071	9.5131	87.8701	.1052	13.4443
(2020 1)	1.019.0 0. (1 1 1) 2UC19UC OUC	(1 1 1)	0 2 19 21	(-.50 .50 0.) (.50 .50 -20.0) (1.00 0. 0.) (-1.0019.00 -2.00)	(.50 .50 -20.0) (-1.0019.00 -2.00)	.7071	20.0125	90.0000	.0500	28.3019

Table 2f

TERRACE ORIENTATION (1 1 0)

MICROFACET EDGE VECTORS TO SERVE AS BASIS VECTORS (-.5 .5 0.) (0. 0. -1.0) (0. -.5 .5)

SURFACE	ALGEBRAIC AND UNIT CELL DECOMPOSITION ON MICROFACETS (1 1 1) (1 1 0) (1 0 0)	STEP NORMAL	ATOM TYPES KINK/ OTHER STEP/ TERRACE/ ALL	TERR EDGE VECT E IN CART. COORD. IN BASIS VECT.S	TERR WIDTH VECT W IN CART. COORD. IN BASIS VECT.S	LENGTH OF E	LENGTH OF W	ANGLE BETWEEN E AND W	SPOT SPLIT- TING	SPOT ROW SPACING TO SPOT SPLITTING RATIO
(2 1 0)	0. 1.0 1.0 (1 0 0) OUC 1UC 1UC	(1 0 0)	0 1 1 2	(0. 0. 1.00) (-.50 1.00 .50) (0. -1.00 0.) (1.00-1.00-1.00)		1.0000	1.2247	65.9052	.8944	1.1180
(3 2 0)	0. 2.0 1.0 (1 0 0) OUC 2UC 1UC	(1 0 0)	0 1 2 3	(0. 0. 1.00) (-1.00 1.50 .50) (0. -1.00 0.) (2.00-1.00-1.00)		1.0000	1.8708	74.4986	.5547	1.8028
(4 3 0)	0. 3.0 1.0 (1 0 0) OUC 3UC 1UC	(1 0 0)	0 1 3 4	(0. 0. 1.00) (-1.50 2.00 .50) (0. -1.00 0.) (3.00-1.00-1.00)		1.0000	2.5495	78.6901	.4000	2.5000
(5 4 0)	0. 4.0 1.0 (1 0 0) OUC 4UC 1UC	(1 0 0)	0 1 4 5	(0. 0. 1.00) (-2.00 2.50 .50) (0. -1.00 0.) (4.00-1.00-1.00)		1.0000	3.2404	81.1236	.3123	3.2016
(6 5 0)	0. 5.0 1.0 (1 0 0) OUC 5UC 1UC	(1 0 0)	0 1 5 6	(0. 0. 1.00) (-2.50 3.00 .50) (0. -1.00 0.) (5.00-1.00-1.00)		1.0000	3.9370	82.7037	.2561	3.9051
(7 6 0)	0. 6.0 1.0 (1 0 0) OUC 6UC 1UC	(1 0 0)	0 1 6 7	(0. 0. 1.00) (-3.00 3.50 .50) (0. -1.00 0.) (6.00-1.00-1.00)		1.0000	4.6368	83.8096	.2169	4.6098
(8 7 0)	0. 7.0 1.0 (1 0 0) OUC 7UC 1UC	(1 0 0)	0 1 7 8	(0. 0. 1.00) (-3.50 4.00 .50) (0. -1.00 0.) (7.00-1.00-1.00)		1.0000	5.3385	84.6259	.1881	5.3151
(9 8 0)	0. 8.0 1.0 (1 0 0) OUC 8UC 1UC	(1 0 0)	0 1 8 9	(0. 0. 1.00) (-4.00 4.50 .50) (0. -1.00 0.) (8.00-1.00-1.00)		1.0000	6.0415	85.2527	.1661	6.0208
(10 9 0)	0. 9.0 1.0 (1 0 0) OUC 9UC 1UC	(1 0 0)	0 1 9 10	(0. 0. 1.00) (-4.50 5.00 .50) (0. -1.00 0.) (9.00-1.00-1.00)		1.0000	6.7454	85.7491	.1487	6.7268
(1110 0)	0. 10.0 1.0 (1 0 0) OUC10UC 1UC	(1 0 0)	0 1 10 11	(0. 0. 1.00) (-5.00 5.50 .50) (0. -1.00 0.) (10.00-1.00-1.00)		1.0000	7.4498	86.1517	.1345	7.4330
(1211 0)	0. 11.0 1.0 (1 0 0) OUC11UC 1UC	(1 0 0)	0 1 11 12	(0. 0. 1.00) (-5.50 6.00 .50) (0. -1.00 0.) (11.00-1.00-1.00)		1.0000	8.1548	86.4848	.1229	8.1394
(1312 0)	0. 12.0 1.0 (1 0 0) OUC12UC 1UC	(1 0 0)	0 1 12 13	(0. 0. 1.00) (-6.00 6.50 .50) (0. -1.00 0.) (12.00-1.00-1.00)		1.0000	8.8600	86.7649	.1130	8.8459
(1413 0)	0. 13.0 1.0 (1 0 0) OUC13UC 1UC	(1 0 0)	0 1 13 14	(0. 0. 1.00) (-6.50 7.00 .50) (0. -1.00 0.) (13.00-1.00-1.00)		1.0000	9.5656	87.0037	.1047	9.5525
(1514 0)	0. 14.0 1.0 (1 0 0) OUC14UC 1UC	(1 0 0)	0 1 14 15	(0. 0. 1.00) (-7.00 7.50 .50) (0. -1.00 0.) (14.00-1.00-1.00)		1.0000	10.2713	87.2098	.0975	10.2591
(1615 0)	0. 15.0 1.0 (1 0 0) OUC15UC 1UC	(1 0 0)	0 1 15 16	(0. 0. 1.00) (-7.50 8.00 .50) (0. -1.00 0.) (15.00-1.00-1.00)		1.0000	10.9772	87.3893	.0912	10.9659
(1716 0)	0. 16.0 1.0 (1 0 0) OUC16UC 1UC	(1 0 0)	0 1 16 17	(0. 0. 1.00) (-8.00 8.50 .50) (0. -1.00 0.) (16.00-1.00-1.00)		1.0000	11.6833	87.5472	.0857	11.6726
(1817 0)	0. 17.0 1.0 (1 0 0) OUC17UC 1UC	(1 0 0)	0 1 17 18	(0. 0. 1.00) (-8.50 9.00 .50) (0. -1.00 0.) (17.00-1.00-1.00)		1.0000	12.3895	87.6871	.0808	12.3794
(1918 0)	0. 18.0 1.0 (1 0 0) OUC18UC 1UC	(1 0 0)	0 1 18 19	(0. 0. 1.00) (-9.00 9.50 .50) (0. -1.00 0.) (18.00-1.00-1.00)		1.0000	13.0958	87.8119	.0764	13.0863
(2019 0)	0. 19.0 1.0 (1 0 0) OUC19UC 1UC	(1 0 0)	0 1 19 20	(0. 0. 1.00) (-9.50 10.00 .50) (0. -1.00 0.) (19.00-1.00-1.00)		1.0000	13.8022	87.9239	.0725	13.7931

Table 2g

Figure Captions

- Fig.1: Some one-dimensional surfaces of two-dimensional crystals and their decomposition into microfacets.
- Fig.2: Relating surface areas and Miller index vectors. The vectors $\vec{u}_0$, $\vec{u}_1$ and $\vec{u}_2$ are perpendicular to the macroscopic surface and the two indicated microfacets, respectively. (The terrace and step are both shown perpendicular to the plane of the figure.)
- Fig.3: The fcc (110) surface. The heavy lines indicate the surface unit cell.
- Fig.4: The fcc (775) stepped surface.
- Fig.5: The fcc (755) stepped surface.
- Fig.6: The fcc (10,8,7) kinked surface, decomposed with two choices of microfacets. For each set of microfacets, the corresponding basis vectors of Eq.31 (the microfacet edge vectors) are shown to the left. The (10,8,7) surface unit cell (Heavy lines) is shown connecting kink atoms.
- Fig.7: Reciprocal lattice of a fcc (10,8,7) surface. Only those lattice points near the terrace diffraction spots, (say, within the drawn ellipses) have appreciable intensity. The quantities a and b are discussed in the text.

XBL794-6172

Fig.1

XBL 794-6171

Fig.2

fcc (110)

XBL794-6166

Fig.3

fcc (775)

XBL 794- 6164

Fig.4

fcc (755)

XBL 796-6398

Fig.5

XBL 794-6165

Fig. 6

XBL 787-5326

Fig.7

This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

Reference to a company or product name does not imply approval or recommendation of the product by the University of California or the U.S. Department of Energy to the exclusion of others that may be suitable.

TECHNICAL INFORMATION DEPARTMENT
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720