

## Step profiles predicted with the modified point-ion model for eight face-centered- and body-centered-cubic surfaces

P. Jiang\* and F. Jona

*College of Engineering and Applied Science, State University of New York at Stony Brook, Stony Brook, New York 11794*

P. M. Marcus

*IBM Research Center, Yorktown Heights, New York 10598*

(Received 20 November 1986)

Calculations of the multilayer relaxation of several open fcc and bcc surfaces have been carried out with the modified point-ion model that was shown earlier to provide satisfactory agreement with experiment for aluminum and iron. The surfaces considered here are the fcc {211}, {311}, {411}, {511}, and the bcc {210}, {310}, {410}, {510}, which have ordered step structures and different roughnesses. The relaxation values are given both in a surface-adapted coordinate system and in the bulk-crystal coordinate system; they are displayed in the form of step-profile distortions. The general trend confirms the edge-atom depression reported earlier by other authors and reveals an overall smoothing of the step profiles.

### I. INTRODUCTION

It has been known for years that the presence of atomic steps on crystal surfaces alters some of the properties of the surfaces in important ways.<sup>1-6</sup> Quantitative understanding of this effect requires knowledge of the structure of the steps and of the associated distortions of the atomic arrangement on the surface with respect to that in the bulk.<sup>7</sup> These distortions are related to the phenomenon of multilayer relaxation of metal surfaces, which has been investigated extensively<sup>8</sup> and is phenomenologically well understood.<sup>9</sup> Direct determinations of step structures (mostly by means of He-atom scattering experiments) have been scarce and contradictory,<sup>10-15</sup> but quantitative information about such step structures can be gathered from the multilayer relaxation data obtained by low-energy electron diffraction<sup>8</sup> (LEED) and, of late, ion-scattering studies.<sup>16</sup> Unfortunately, these data are also relatively scarce, so that general conclusions about distortions from ideal step profiles cannot yet be drawn with confidence. However, these distortions can be reliably calculated with the theory based on the point-ion model recently introduced.<sup>9</sup> This model is a modification of the simple electrostatic model originally proposed by Finnis and Heine<sup>17</sup> in order to explain the contraction of the first interlayer spacing observed on many metal surfaces. The modification consists of an increase of the force that binds each ion to its bulk position over the force due to a uniform distribution of electronic charge. The magnitude of the increase can be fixed empirically for each bulk structure.<sup>9</sup> Calculations made with this model were shown to reproduce well the multilayer relaxations determined by LEED on six surfaces of bcc Fe and six of fcc Al.<sup>9</sup> Exploiting the so-tested predictive power of the model, we have calculated in the present work the multilayer relaxation of eight surfaces of two metal structures in which Miller indices systematically increase, namely, fcc {211}, {311}, {411},

{511}, and bcc {210}, {310}, {410}, and {510}. This particular choice of Miller indices was motivated by the fact that these surfaces form systematic sequences of increasing openness in which some members were already successfully compared with experiment.<sup>8,9</sup> The calculations yield the atomic shifts from bulk positions expected in the first five or six layers at the surface and are found initially in terms of the surface coordinate system. By converting these shifts into the coordinate system of the cubic unit cell we are in a position to depict the distortions from "bulklike" step profiles on all surfaces studied. These theoretical predictions should be experimentally tested, but the fact that similar calculations produced substantial agreement with a large set of experimental data<sup>9</sup> makes plausible that these predictions are meaningful, and should provide guidance to new work on stepped surfaces, not only by LEED but also by other techniques, e.g., ion scattering and atom diffraction.

In Sec. II we summarize the method used for the calculations, and in Sec. III we present and discuss the results.

### II. METHOD OF CALCULATION

Details of the modified point-ion model and of the procedures used for calculations of surface relaxations are given in our earlier paper.<sup>9</sup> Here we give for the convenience of the reader a brief outline of the calculational procedure. We consider a semi-infinite metal crystal consisting of neutral layers with thickness  $d$ . Each layer contains a two-dimensional net of positive ions imbedded in a slab of uniform electron gas. The slab of negative charge is rigid; the ion nets can translate rigidly. In the bulk each net is in the center of the corresponding slab while in the surface a net is usually displaced from the center of its slab (surface relaxation). This displacement is a consequence of the electrostatic forces that are created when the solid is truncated. The displacement is fixed by a bal-

TABLE I. Surface-adapted lattice vectors. All entries are in units of  $a$ , the side of the cubic cell. Primitive vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  and axes  $x$  and  $y$  are in the surface plane;  $x$  is along  $\mathbf{a}_1$  (direction given as  $[x]$ ); rotation counterclockwise from  $\mathbf{a}_1$  to  $\mathbf{a}_2$  gives  $y$  at  $90^\circ$  (direction given by  $[y]$ ) and  $\mathbf{a}_2$  at  $\theta_{12}$  (in degrees);  $z$  is then into the paper (left-handed coordinate system) and into the crystal;  $\mathbf{a}_3$  is a primitive vector (components  $a_{3x}$ ,  $a_{3y}$ , and  $a_{3z}$ ) between adjacent layers parallel to the surface plane.

Surface	$a_1$	$[x]$	$a_2$	$[y]$	$\theta_{12}$	$a_{3x}$	$a_{3y}$	$a_{3z}=d$
fcc{211} <sup>a</sup>	$1/\sqrt{2}$	$[01\bar{1}]$	$\sqrt{3}$	$[\bar{1}11]$	90.0	$1/2\sqrt{2}$	$1/\sqrt{3}$	$1/2\sqrt{6}$
fcc{311} <sup>a</sup>	$1/\sqrt{2}$	$[01\bar{1}]$	$\sqrt{3}/2$	$[\bar{2}33]$	106.8	$1/2\sqrt{2}$	$5/2\sqrt{22}$	$1/\sqrt{11}$
fcc{411} <sup>a</sup>	$1/\sqrt{2}$	$[01\bar{1}]$	3	$[\bar{1}22]$	90.0	$1/2\sqrt{2}$	$7/6^b$	$1/6\sqrt{2}$
fcc{511}	$1/\sqrt{2}$	$[01\bar{1}]$	$\sqrt{7}/2$	$[\bar{2}55]$	100.9	$1/2\sqrt{2}$	$17/6\sqrt{6}$	$1/3\sqrt{3}$
bcc{210} <sup>a</sup>	1	$[00\bar{1}]$	$\sqrt{5}$	$[\bar{1}20]$	90.0	1/2	$3/2\sqrt{5}^b$	$1/2\sqrt{5}$
bcc{310} <sup>a</sup>	1	$[001]$	$\sqrt{11}/2$	$[\bar{1}30]$	107.5	0	$3/\sqrt{10}$	$1/\sqrt{10}$
bcc{410}	1	$[00\bar{1}]$	$\sqrt{17}$	$[\bar{1}40]$	90.0	1/2	$13/2\sqrt{17}$	$1/2\sqrt{17}$
bcc{510}	1	$[00\bar{1}]$	$\sqrt{27}/2$	$[\bar{1}50]$	101.1	1/2	$4\sqrt{2}/13$	$1/\sqrt{26}$

<sup>a</sup>These surface-adapted vectors appear also in J. F. Nicholas, *An Atlas of Models of Crystal Systems* (Gordon and Breach, New York, 1965). Nicholas chooses positive  $z$  out of the paper and out of the crystal (opposite to our convention), and gives lengths in units of  $a/2$ .

<sup>b</sup>The  $x$  and  $y$  directions used for this surface here and in later tables are opposite to those used by Nicholas, and  $a_{3y}$  is different.

TABLE II. Absolute and relative relaxations in surface coordinates.  $\Delta R_{iy}$  and  $\Delta R_{iz}$  give the absolute movement from bulk positions along the  $y$  and  $z$  directions defined in Table I of atoms in the  $i$ th layer;  $\Delta R_{ix}$  vanishes by symmetry for all surfaces considered here;  $\Delta a_{i,i+1,y} = \Delta R_{i+1,y} - \Delta R_{i,y}$  is the relative change in  $y$  position of the  $(i+1)$ st layer with respect to the  $i$ th;  $\Delta d_{i,i+1} = \Delta R_{i+1,z} - \Delta R_{i,z}$  is the increase in the  $i$ th spacing due to relaxation.

$i$	Relaxation		Percentage relaxation		Relaxation		Percentage relaxation	
	$\frac{\Delta R_{iy}}{d}$	$\frac{\Delta R_{iz}}{d}$	$\frac{\Delta a_{i,i+1,y}}{a_{3y}}$	$\frac{\Delta d_{i,i+1}}{d}$	$\frac{\Delta R_{iy}}{d}$	$\frac{\Delta R_{iz}}{d}$	$\frac{\Delta a_{i,i+1,y}}{a_{3y}}$	$\frac{\Delta d_{i,i+1}}{d}$
			fcc{211}				fcc{311}	
1	-0.40	0.21	19.0	-23.0	-0.05	0.09	3.7	-12.2
2	0.14	-0.02	-9.8	-1.5	0.01	-0.03	-1.4	4.4
3	-0.14	-0.04	6.1	5.2	-0.01	0.01	0.5	-1.7
4	0.03	0.02	-1.3	-1.5	0.00	0.00	-0.1	0.6
5	0.00	0.00	0.7	-0.7	0.00	0.00	0.1	-0.2
6	0.02	-0.01			0.00	0.00		
			fcc{411}				fcc{511}	
1	-0.02	0.52	4.6	-36.2	0.16	0.24	-6.5	-26.6
2	0.43	0.16	-12.1	-21.3	-0.23	-0.02	7.0	-1.3
3	-0.77	-0.06	12.2	2.9	0.19	-0.04	-4.7	4.3
4	0.44	-0.03	-3.3	-5.9	-0.09	0.01	1.6	0.7
5	0.11	-0.09	-3.7	12.3	0.01	0.01	-0.3	-3.0
6	-0.25	0.04			-0.01	-0.02		
			bcc{210}				bcc{310}	
1	-0.41	0.25	22.5	-22.0	0.07	0.13	-5.9	-16.8
2	0.26	0.03	-7.9	-9.8	-0.11	-0.03	4.8	4.2
3	0.03	-0.07	-2.1	10.5	0.04	0.01	-1.6	-1.5
4	-0.04	0.04	2.2	-4.7	-0.01	-0.01	0.5	1.1
5	0.03	-0.01	-0.9	0.8	0.00	0.00	-0.3	-0.6
6	0.00	0.00			0.00	0.00		
			bcc{410}				bcc{510}	
1	-0.10	0.56	3.1	-37.4	0.07	0.34	-5.1	-31.5
2	0.29	0.29	-9.9	-29.4	-0.34	0.02	8.7	-6.7
3	-0.99	0.00	12.5	1.9	0.35	-0.05	-7.1	4.2
4	0.64	0.02	-2.1	-16.3	-0.22	0.00	2.3	2.0
5	0.37	-0.15	-7.5	15.3	-0.03	0.01	0.2	-3.5
6	-0.60	0.01			-0.02	-0.02		

TABLE III. Component and total relaxations of cubic coordinates.  $\Delta R_{ix'}$ ,  $\Delta R_{iy'}$ , and  $\Delta R_{iz'}$  are the absolute movements of relaxed atoms in the  $i$ th layer from bulk positions along the cubic axes [ $x'$ ]=[100], [ $y'$ ]=[010], [ $z'$ ]=[001];  $\Delta R_i$  is the total magnitude of the movement of the  $i$ th layer atom; the vectors  $\Delta \mathbf{R}_i$  are plotted in the figures.

$i$	$\frac{\Delta R_{ix'}}{d}$	$\frac{\Delta R_{iy'}}{d}$	$\frac{\Delta R_{iz'}}{d}$	$\frac{\Delta R_i}{d}$	$\frac{\Delta R_{ix'}}{d}$	$\frac{\Delta R_{iy'}}{d}$	$\frac{\Delta R_{iz'}}{d}$	$\frac{\Delta R_i}{d}$
	fcc{211}				fcc{311}			
1	0.06	-0.32	-0.32	0.46	-0.06	-0.06	-0.06	0.10
2	-0.06	0.09	0.09	0.14	0.02	0.02	0.02	0.03
3	0.11	-0.07	-0.07	0.14				
	fcc{411}				fcc{511}			
1	-0.48	-0.14	-0.14	0.52	-0.28	0.06	0.06	0.29
2	-0.29	0.25	0.25	0.46	0.08	-0.15	-0.15	0.23
3	0.31	-0.50	-0.50	0.77	-0.02	0.14	0.14	0.20
4	-0.12	0.30	0.30	0.44	0.02	-0.06	-0.06	0.09
5	0.04	0.10	0.10	0.15				
6	0.05	-0.18	-0.18	0.26				
	bcc{210}				bcc{310}			
1	-0.41	0.26	0.00	0.49	-0.11	-0.11	0.00	0.16
2	0.09	-0.25	0.00	0.27	0.00	0.11	0.00	0.11
3	0.07	0.01	0.00	0.07	0.00	-0.04	0.00	0.04
4	-0.05	0.02	0.00	0.05				
	bcc{410}				bcc{510}			
1	-0.62	-0.26	0.00	0.67	-0.34	0.00	0.00	0.34
2	-0.35	0.22	0.00	0.41	0.05	-0.34	0.00	0.34
3	0.24	-0.96	0.00	0.99	-0.02	0.36	0.00	0.36
4	-0.17	0.62	0.00	0.64	0.05	-0.21	0.00	0.22
5	0.05	0.39	0.00	0.39				
6	0.14	-0.59	0.00	0.61				

ance between the force within each layer that tries to keep the ion net in its bulk position and the force due to interactions with other layers that depend on relative positions of the nets. The final configuration is the one that reduces the forces acting on the nets to zero or, equivalently, minimizes the electrostatic energy. Thus the relaxed structure is obtained by minimizing the energy as a function of the position vectors of the nets. We introduce an empirical factor  $\alpha$  which increases the restoring force pulling the net to the center of its slab and which has been set equal to 1.9 in the earlier calculations<sup>9</sup> (and

used in the present calculations). This value fits the data on Fe and Al well and is not far off for Cu, hence it is suitable to illustrate the behavior of interest.

The actual energy expression which is minimized with respect to the structural parameters can be written as

$$E = \alpha \sum_{j=1}^{\infty} E_1(O_{jz}) + \sum_{j=1}^{\infty} \sum_{k>j} E_2(\mathbf{O}_j, \mathbf{O}_k),$$

where the  $\mathbf{O}_j$  vectors (components  $O_{jp}$ ,  $O_{jz}$ ) are position vectors of an origin atom in the  $j$ th layer referred to an origin atom in the first layer as overall origin. Then

TABLE IV. Atomic displacements from bulk positions.  $\Delta R_i$  denotes the magnitude of displacements of  $i$ th layer atom in the relaxed lattice from the bulk position;  $r_b$  denotes the bulk atomic radius;  $\Delta R_{iz}$  denotes the  $z$  component of displacement of  $i$ th layer atom (positive  $z$  into the crystal).

Surface	Roughness <sup>a</sup>	$\frac{\Delta R_1}{r_b}$	$\frac{\Delta R_{1z}}{r_b}$	$\frac{\Delta R_2}{r_b}$	$\frac{\Delta R_{2z}}{r_b}$	$\frac{\Delta R_3}{r_b}$	$\frac{\Delta R_{3z}}{r_b}$
		fcc{211}	3.2	0.27	0.12	0.08	-0.01
fcc{311}	2.1	0.09	0.08	0.03	-0.03		
fcc{411}	5.4	0.17	0.17	0.15	0.05	0.26	-0.02
fcc{511}	3.3	0.16	0.13	0.13	-0.01	0.11	-0.02
bcc{210}	3.8	0.25	0.13	0.14	0.02	0.04	-0.04
bcc{310}	2.7	0.12	0.09	0.08	-0.02	0.03	0.01
bcc{410}	7.0	0.19	0.16	0.11	0.08	0.28	0.00
bcc{510}	4.3	0.15	0.15	0.15	0.01	0.16	-0.02

<sup>a</sup>Reference 18.

$$E_1(O_{jz}) = (2\pi Z^2 / \mathcal{A}d) [O_{jz} - (j - 1/2)d]^2$$

is the change in electrostatic energy of the  $j$ th layer from the bulk value when the net is displaced from the center of the slab;  $Z$  is the effective charge on each ion,  $\mathcal{A}$  is the unit mesh area, and  $d$  is the bulk spacing. The second term,

$$E_2(O_j, O_k) = (2\pi Z^2 / \mathcal{A}) \sum_h \{ \exp[ i \mathbf{K}_h \cdot (O_{jp} - O_{kp}) - K_h | O_{kz} - O_{jz} | ] / K_h \},$$

is a Fourier expansion of the electrostatic energy of the

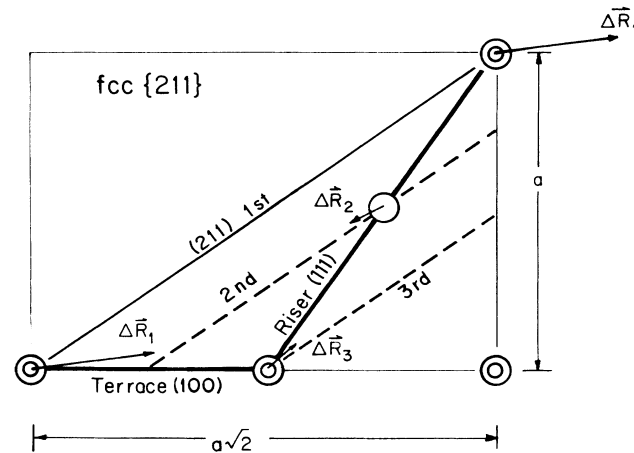
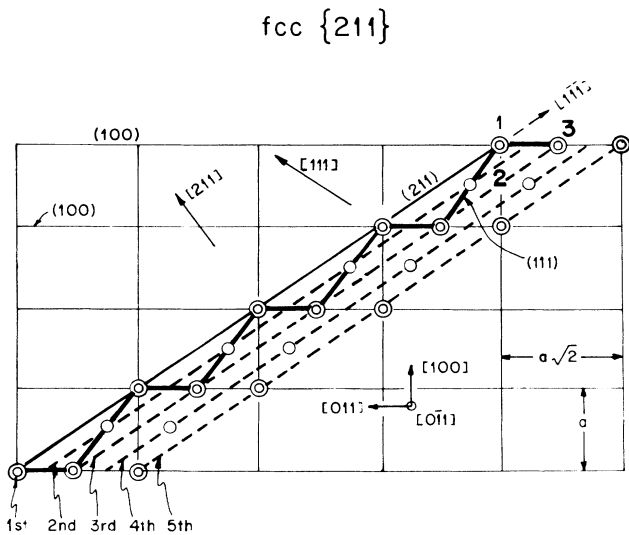


FIG. 1 fcc{211} surface. Upper panel: overall step profile of bulk-terminated (unrelaxed) surface. Atoms are numbered according to the layer (first, second, etc.) in which they are located. Lower panel: magnified detail of the surface relaxation. The arrows represent atomic shifts and are four times larger than required in order to be to scale with the size of the lattice parameter  $a$ . All  $\Delta R_i$  are parallel to  $\{110\}$ . Atoms in the plane of the figure are indicated by double circles; atoms above or below the plane of the figure by single circles.

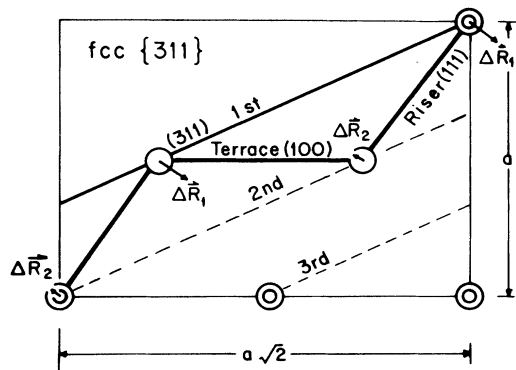
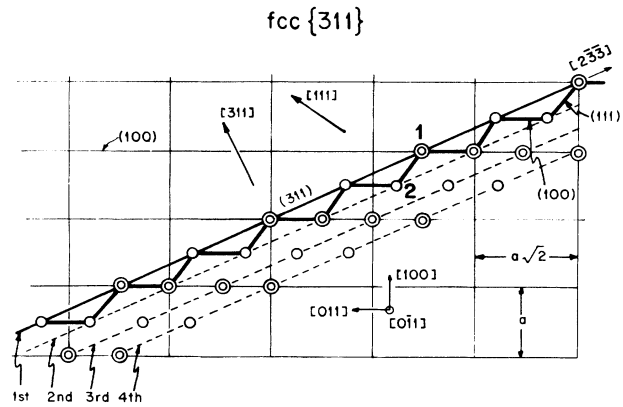


FIG. 2. fcc{311} surface. See caption to Fig. 1.

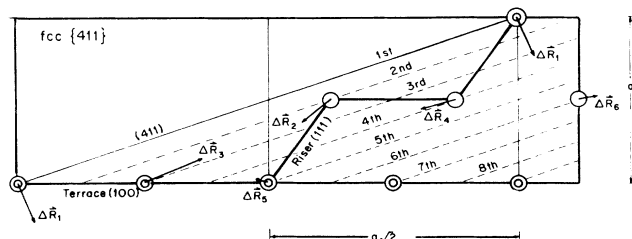
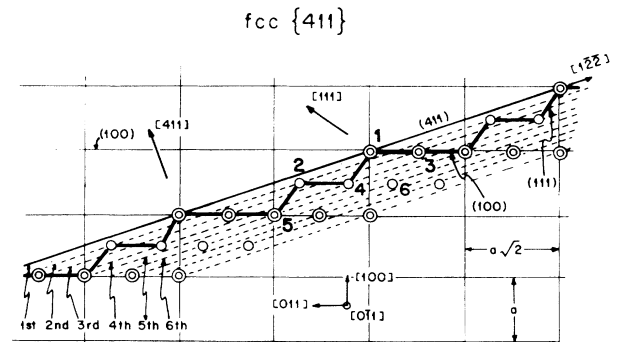


FIG. 3. fcc{411} surface. See caption to Fig. 1.

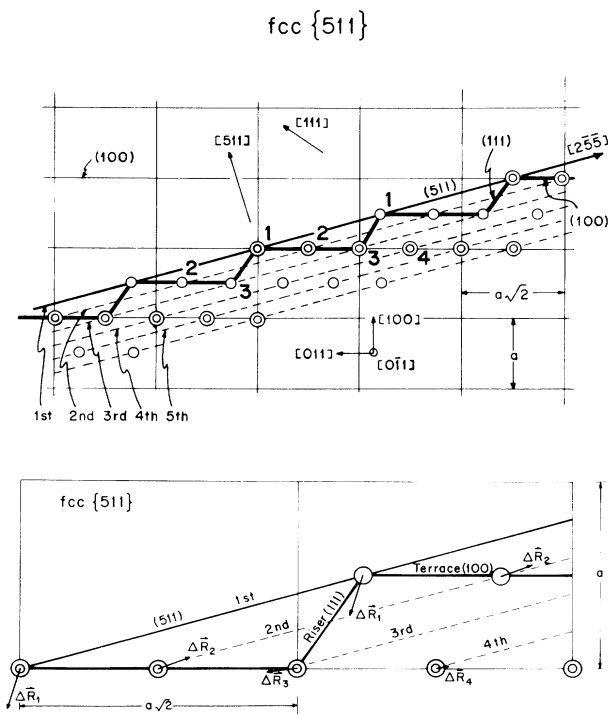


FIG. 4. fcc{511} surface. See caption to Fig. 1.

$j$ th and  $k$ th (neutral) layers. The wave vectors  $\mathbf{K}_h = 2\pi(h_1\mathbf{b}_1 + h_2\mathbf{b}_2)$ , where  $\mathbf{b}_1$  and  $\mathbf{b}_2$  are primitive vectors of the reciprocal lattice of the net, have magnitude  $K_h$ , and the sum is over all reciprocal-lattice vectors except  $h_1 = h_2 = 0$ .

The relaxed values of the structural parameters  $\mathbf{O}_j$  are obtained by minimizing  $E/(2\pi Z^2 d/\mathcal{A})$  as a function of the  $\mathbf{O}_j$  for all  $j$ ; the values of  $\mathbf{K}_h$ ,  $\mathcal{A}$ , and  $d$  are fixed by the bulk geometry; the structure is independent of  $Z$ , which does not need to be specified. The expansion has exponential convergence in the separation distance between layers  $j$  and  $k$ , hence convergence is slower for more open surfaces, e.g., 18 terms are needed for fcc{001}, 11 terms for bcc{011}, 34 for bcc{001}, 142 for fcc{211}, 197 for fcc{511}, 214 for bcc{210}, and 378 for bcc{510} to maintain four significant figures.

### III. RESULTS AND DISCUSSIONS

The lattice vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ , and  $\mathbf{a}_3$  for each of the eight surfaces considered here are given in Table I, which also relates the surface coordinate system  $x, y, z$  to the cubic axes. The results of the relaxation calculations for each surface are presented in different forms in the following tables and figures. Table II gives the absolute and relative relaxations in the surface coordinate system  $x, y, z$ . Table III gives the component and total relaxations in the cubic coordinate system  $x' = [100]$ ,  $y' = [010]$ ,  $z' = [001]$ . Table IV summarizes for each surface the roughness value<sup>18</sup> and the atomic displacements in the first three layers. Both the magnitude of these displacements and their components in the  $z$  direction (into the crystal perpendicular

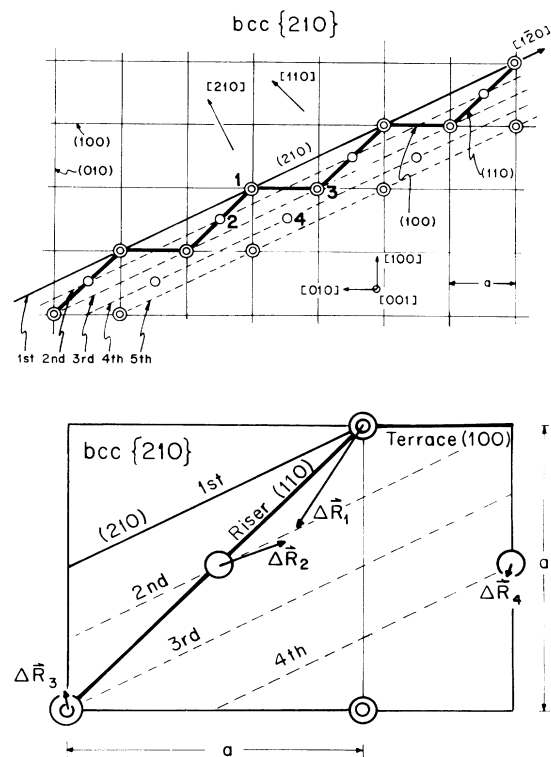
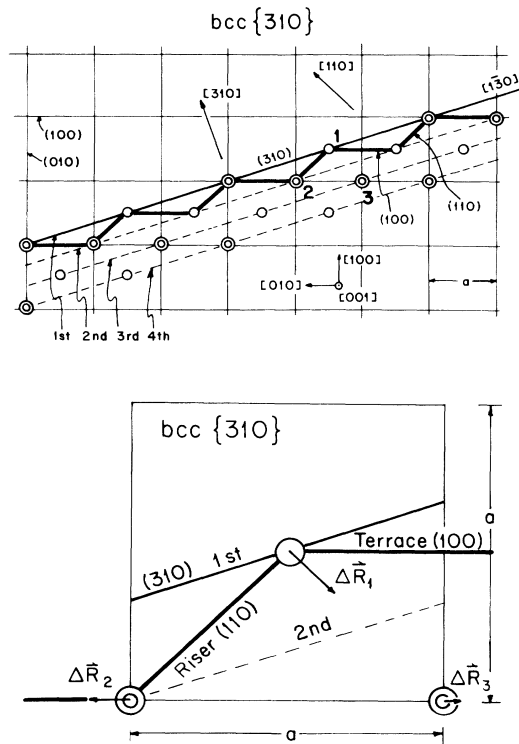
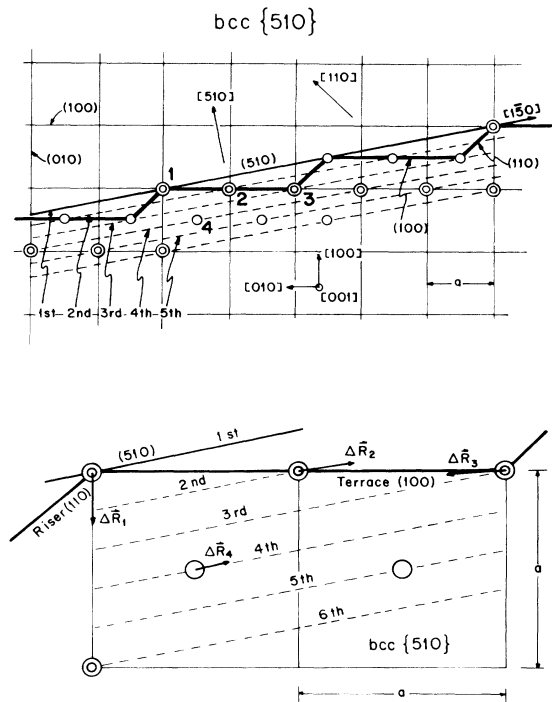


FIG. 5 fcc{210} surface. Upper panel: overall step profile of bulk-terminated (unrelaxed) surface. Atoms are numbered according to the layer (first, second, etc.) in which they are located. Lower panel: magnified detail of the surface relaxation. The arrows represent atomic shifts and are four times larger than required in order to be to scale with the size of the lattice parameter  $a$ . All  $\Delta R_i$  are parallel to {100}. Atoms in the plane of the figure are indicated by double circles; atoms above or below the plane of the figure by single circles.

to the surface) are given in terms of the bulk atomic radius  $r_b$ . One can then compare directly the absolute displacements of the atoms in different layers, on different surfaces and for the two lattices (fcc and bcc), and find the displacement magnitudes ( $r_b = 1.24$  Å for Fe,  $r_b = 1.43$  Å for Al). Note that the edge atoms, which are generally first-layer atoms, have substantial perpendicular components of displacement whereas the interior atoms of the step have primarily parallel components, which can be large (see, e.g., the third layer in fcc{411} and bcc{410}). The fcc{411} and bcc{410} surfaces have second-layer edge atoms as well, and these also show substantial perpendicular displacements.

The steplike character of each surface and the distortion thereof are shown graphically in the Figs. 1–8. In each figure, we present in the upper panel an overall cross-sectional view of the unrelaxed surface perpendicular to the  $x$  direction, with the step profile emphasized by thick lines. Atoms in successive layers are numbered successively (e.g., 1, 2 on fcc{211}, etc.). Atoms in the plane of the paper are drawn as double circles, atoms above or below the plane of the paper as single circles: the latter

FIG. 6.  $\text{bcc}\{310\}$  surface. See caption to Fig. 5.FIG. 8.  $\text{bcc}\{510\}$  surface. See caption to Fig. 5.

atoms are, for the fcc surfaces,  $a\sqrt{2}/4$ ; for the bcc surfaces,  $a/2$  above or below the plane of the drawing.

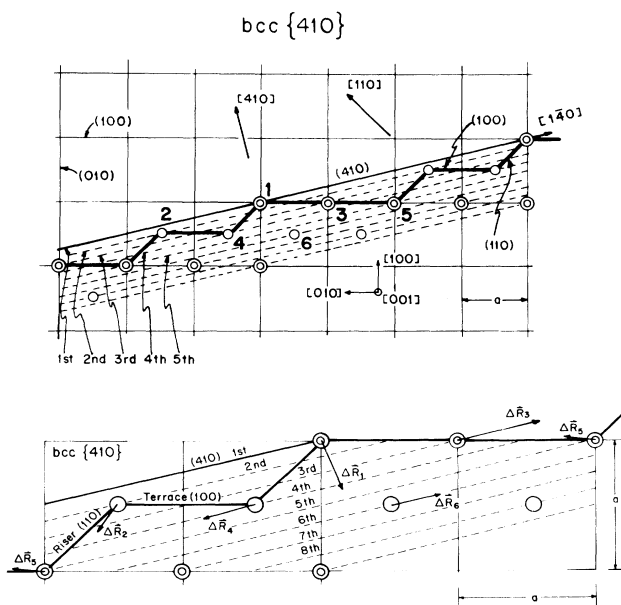
The lower panel in each figure depicts a magnified detail of the overall cross-sectional view and the shifts that the surface atoms suffer because of the relaxation. These shifts are denoted with the vectors  $\Delta\vec{R}_i$  (listed in Table

III), where  $i$  is the number of the corresponding atom in the overall cross-sectional view. Two important points should be noted about these shifts. One is that arrows have been drawn *only for these shifts that are larger than  $0.01a$* . The other is that *the arrows have been drawn four times longer than would be required for them to be to scale with the rest of these magnified details*. This further magnification was found to be necessary in order to make the shortest arrows visible at all, especially after reduction for printing. We note that for all eight surfaces studied here all shifts are parallel to the plane of the drawing and perpendicular to the step edges.

These magnified details are meant to depict the distortions of the step profiles. The trend seems to be in the direction of reducing the step height, in qualitative agreement with Henzler's edge-atom depression,<sup>6</sup> and smoothing the sharp edge profile. This trend is consistent with the results of calculations by Allan<sup>19</sup> for the  $\text{Pt}\{233\}$  and the  $\text{Pt}\{650\}$  surfaces. As mentioned in the Introduction, only for some of the surfaces studied here are experimental data available (by LEED), but it is hoped that the present results will help and stimulate ion-scattering and atom-diffraction workers toward determining step-profile distortions.

#### ACKNOWLEDGMENTS

Two of the authors (P.J. and F.J.) would like to express appreciation for partial support of this work by the National Science Foundation with Grant No. DMR8301165A01.

FIG. 7.  $\text{bcc}\{410\}$  surface. See caption to Fig. 5.

- \*On leave from the Physics Department, Fudan University, Shanghai, People's Republic of China.
- <sup>1</sup>W. R. Burton, N. Cabrera, and F. C. Frank, *Philos. Trans. R. Soc. London, Ser. A* **243**, 299 (1951).
- <sup>2</sup>B. Lang, R. W. Joyner, and G. A. Somorjai, *Surf. Sci.* **30**, 454 (1972); C. Zhang, A. J. Gellman, G. J. Wang, and G. A. Somorjai, *ibid.* **164**, L835 (1985).
- <sup>3</sup>R. W. Joyner, B. Lang, and G. A. Somorjai, *J. Catal.* **27**, 405 (1972); L. M. Falicov and G. A. Somorjai, *Proc. Natl. Acad. Sci. U.S.A.* **82**, 2207 (1985); D. R. Strongin, J. Carrazza, S. R. Bare, and G. A. Somorjai (unpublished).
- <sup>4</sup>K. Besocke and H. Wagner, *Phys. Rev. B* **8**, 4597 (1973); *Surf. Sci.* **53**, 351 (1975).
- <sup>5</sup>M. Henzler, and J. Clabes, *Jpn. J. Appl. Phys., Suppl. 2, Part 2*, 389 (1974).
- <sup>6</sup>M. Henzler, *J. Appl. Phys.* **40**, 3758 (1969).
- <sup>7</sup>J. M. Blakely and R. L. Schwebel, *Surf. Sci.* **26**, 321 (1971).
- <sup>8</sup>See, e.g., D. L. Adams and C. S. Sorensen, *Surf. Sci.* **166**, 495 (1986), and references given therein.
- <sup>9</sup>P. Jiang, P. M. Marcus, and F. Jona, *Solid State Commun.* **59**, 275 (1986).
- <sup>10</sup>M. Henzler, *Surf. Sci.* **19**, 159 (1970); *Appl. Phys.* **9**, 11 (1976).
- <sup>11</sup>K. Besocke and H. Wagner, *Surf. Sci.* **52**, 653 (1975).
- <sup>12</sup>R. Kaplan, *Surf. Sci.* **93**, 145 (1980).
- <sup>13</sup>G. Comsa, G. Mechttersheimer, B. Poelsema, and S. Tomoda, *Surf. Sci.* **89**, 123 (1979).
- <sup>14</sup>J. Lapujoulade and Y. Lejay, *Surf. Sci.* **69**, 354 (1977).
- <sup>15</sup>D. Gorse, B. Salanon, F. Fabre, A. Kara, J. Perreau, G. Armand, and J. Lapujoulade, *Surf. Sci.* **147**, 611 (1984).
- <sup>16</sup>M. Copel and T. Gustaffson, *Bull. Am. Phys. Soc.* **31**, 323 (1986); T. Gustaffson, M. Copel, W. R. Graham, and S. M. Yalisove, *ibid.* **31**, 324 (1986); S. M. Yalisove, W. R. Graham, M. Copel, and T. Gustaffson *ibid.* **31**, 325 (1986).
- <sup>17</sup>M. W. Finnis and V. Heine, *J. Phys. F* **4**, L37 (1974).
- <sup>18</sup>The surface roughness is defined as the inverse of the fraction of the area in the surface plane occupied by atoms of radius equal to one-half the bulk nearest-neighbor distance (the bulk radius).
- <sup>19</sup>G. Allan, *Surf. Sci.* **85**, 37 (1979); **89**, 142 (1979).