TABLE II. Interstitial cluster size.

F-Center decay rate at 30°C (centers/MeV sec)		Ratio of rates	Number of interstitials per cluster	
During aggregation	During annihilation		Assume equal cross section	Assume geometric cross section
$(9\pm1)\times10^3$	$(2\pm\frac{1}{2})\times10^2$	~50	~35	~200

appears to be more reasonable. Table II gives the values for the size of the interstitial clusters for irradiation in the vicinity of room temperature obtained using these assumptions. Clearly even for comparable interaction radii the results imply rather large clusters.[35]

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[35] These estimates are based on the assumption that random diffusion controls both the annihilation and aggregation of nega-

ACKNOWLEDGMENTS

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tive-ion vacancies. If M-center formation were due, for example, to highly correlated combination of nearby F centers [see, e.g., Y. Farge, M. Lambert, and R. Smoluchowski, Solid State Commun. **4**, 333 (1966)], then the above comparison would be invalid.

Interaction Potentials of Gas Atoms with Cubic Lattices on the 6-12 Pairwise Model

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The interaction potential energy of a gas atom with a solid is obtained by summing the 6-12 gas-atom–solid-atom pairwise potential over all atoms of a perfect, monatomic, cubic, semi-infinite lattice model. Study is made of relations among (i) heats of adsorption, surface diffusion, and sublimation; (ii) lattice spacing, lattice type [body-centered and face-centered cubic], and exposed lattice face [(100) and (110)]; and (iii) the pairwise interaction parameters. Possibilities of obtaining one or more of these quantities from knowledge of the others are considered. The theory is applied to an analysis of experimental data, and a somewhat unsuccessful attempt is made to assess the validity of the 6-12 pairwise model in gas-surface interactions. Tables, correct to five significant figures, of sums of inverse sixth and twelfth powers of gas-atom–solid-atom distances are presented as functions of distance of the gas atom from the surface of a simple cubic lattice which has either its (100) or its (110) face exposed.

I. INTRODUCTION

EXAMINATION is made of the assumption that the interaction of a gas atom with a solid may be described by means of a potential energy obtained by a summation over all atoms of the solid of the Lennard-Jones 6-12 gas-atom–solid-atom pairwise interaction potential[1]:

$$V_{ij}/\epsilon = (r_0/r_{ij})^{12} - 2(r_0/r_{ij})^6. \qquad (1)$$

V_{ij} is the potential energy of interaction of atoms i and j separated by a distance r_{ij}; r_0 and ϵ are the 6-12 gas-atom–solid-atom parameters, the physical significance of which is well known. The solid is represented by a perfect, monatomic, cubic, semi-infinite lattice model, and the interaction potential of a gas atom near the surface is assumed to be obtained by summing (1)

over all atoms j of the semi-infinite lattice with $i=$ gas atom.

The lattice type is denoted by L, and a notation of Born[2] is used: L=s, b, and f denote, respectively, the simple, body-centered and face-centered cubic lattices. The lattice spacing is a (the nearest-neighbor distances are $q^{\frac{1}{2}}a/2$, where $q=4$, 3, and 2, respectively, for s, b, and f lattices). The exposed face F of the lattice must be specified [F=(110), for example] and the notation used is that FL means the F face of the L lattice; the conventional round brackets in the face specification are omitted hereafter (for example, F=110).

Questions to which we attempt partial answers are the following:

(1) What is the atomic heat H of adsorption at zero coverage and the corresponding "heat" (activation

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[1] J. E. Lennard-Jones, Physica **4**, 941 (1937).

[2] M. Born, Proc. Cambridge Phil. Soc. **36**, 160 (1940).

energy) D of surface diffusion as functions of r_0, ϵ, a, L, and F?

(2) What does a topographical "map" of the gas-surface interaction potential energy look like as a function of these quantities?

(3) What may be deduced about r_0, ϵ, and F from studies of H and D and from other studies, for example the scattering of gas atoms by a clean surface of known material (and hence of known a and L, but not in general of known F)?

Discussion of previous relevant work is delayed until after various definitions have been made. The analogous situation for infinite lattices (for which surface effects are negligible compared to bulk effects) is simpler, and we need some of the results; therefore, a brief discussion may not be out of place.

Infinite Lattices

In this case, V_{ij} is the solid-atom–solid-atom pairwise interaction potential; r_0 and ϵ are the solid-atom–solid-atom parameters. The assumption is that the crystal potential energy is obtained by a summation of (1) over the infinite lattice, and that the bulk properties of crystals are derivable from this potential energy. In this way, *all* bulk properties (including, for example, crystal structure) are functions only of r_0 and ϵ.

Work of this nature has been done by many authors[1-20] using many pairwise interaction laws, both of type (1) and others; for example,[19,20] the Morse potential.[21] A detailed discussion of the various pairwise interaction laws and of their relations with the relevant experimental data is found in Ref. 22; a review of the solid-state work appears in Ref. 23. For the purposes of this discussion, it is sufficient to note that r_0 and ϵ are determined by four experimental quantities, (i) the

atomic volume v at zero p and T, (ii) the atomic heat λ of sublimation at zero p and T, (iii) the atomic zero-point energy E_0 at zero p and (iv) L. [Because of stability considerations,[2,4,7,23] (1) cannot hold for b or s lattices, although it is used[8] for crystals of both types f and b in the hope that it yields a useful model for a description of many crystal properties; s crystals are unknown in nature.[24]] Knowledge of v and L implies knowledge of a and, when E_0 is negligible, r_0/a and ϵ/λ are functions only of L. (Corrections to be applied when E_0 is not negligible are discussed by Corner.[6]) In fact, it may be shown from the work of Refs. 4 and 7 that

$$r_0/a \simeq 0.7280 \text{(f)}, \quad 0.9099 \text{(b)}, \qquad (2a)$$

and

$$\epsilon/\lambda \simeq 0.1161 \text{(f)}, \quad 0.1213 \text{(b)}. \qquad (2b)$$

Semi-Infinite Lattices

The problem of the interaction of a gas atom with a semi-infinite lattice is more complicated than the infinite-lattice problem because of the extra parameters which must be specified. Briefly, a result is that, when zero-point energy is neglected, the reduced gas-atom–solid-atom parameter r_0/a is determined in general by H/D, L, and F; ϵ is then determined by either H or D.

Semi-infinite lattice sums are defined by

$$S_k(\text{FL},x,y,z) = \sum_j (a/r_{ij})^k, \qquad (3)$$

where r_{ij} is the distance of the jth lattice point from the gas atom i, which is located at the point (x,y,z). The potential energy $V(\text{FL},x,y,z,r_0/a,\epsilon)$ of the gas atom is therefore given by

$$
V(\text{FL},x,y,z,r_0/a,\epsilon)/\epsilon
$$
$$
= (r_0/a)^6[(r_0/a)^6 S_{12}(\text{FL},x,y,z) - 2S_6(\text{FL},x,y,z)]. \quad (4)
$$

Two important approximations (inherent also in all previous work on semi-infinite lattice sums but not always clearly stated) are made; these are that the lattice remains undistorted in spite of the presence of both (i) the free surface and (ii) the gas atom. These approximations result in such great simplifications of the calculations that it is worthwhile to make them at this stage of the theory.

One such simplification is that results for both Fb and Ff faces may then be obtained by superposition of appropriate results for the Fs face; therefore detailed sums are done only for the s lattice. In order that results on at least two different faces may be compared, calculations are made for F=110 and 100.[25] For b, f, and s lattices, these faces are shown, respectively, in Figs. 1 and 2, together with x and y axes defining right-handed systems of rectangular cartesian coordi-

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[25] Remember that we are using the notation 110=(110), 100=(100), etc.

nates, the surface planes (containing the surface atom centers) being $z=0$.

Adsorption and surface-diffusion properties are determined by the equilibrium position with respect to z of a gas atom located directly above the point (x,y) on the surface, and by the value of the interaction potential at this position. $z_m(\mathrm{FL},x,y,r_0/a)$ is the value of z making $V(\mathrm{FL},x,y,z,r_0/a,\epsilon)$ a minimum V_m, with respect to z:

$$V(\mathrm{FL},x,y,z_m,r_0/a,\epsilon)=V_m(\mathrm{FL},x,y,r_0/a,\epsilon). \qquad (5)$$

An important problem in gas-surface interactions concerns the "smoothness" of the surface potential "seen" by an incident gas atom. The hard-cubes scattering theory of Logan and Stickney[26] assumes a perfectly smooth surface (although surface roughness is considered later[27]), whereas the hard-spheres theory of the author[28,29] assumes relatively rough surfaces. The theory of Oman and his co-workers[30–33] uses the same gas-surface potential function as that in this paper, and from this point of view this paper is an investigation into the surface properties of that theory. In both the hard-cubes[26,27] and hard-spheres[28,29] models the incident gas atom may be thought of as a point mass, and the surface as an array of hard spheres of radius R; in the former theory $R=\infty$ and in the latter $R\simeq1.1a$ (for inert-gas-W systems). The hard-cubes model is far more successful in describing recent low-incident-energy narrow-lobe gas-surface scattering patterns[34–36] than is the author's. That the author's model cannot adequately describe these patterns should cause no surprise, as it is developed specifically for high incident energies; that the hard-cubes model *does* describe the patterns so well (at least, qualitatively) is, however, surprising.[27] Logan and Stickney[26] state that partial justification for their smooth-surface assumption is provided by a discussion of potentials by Ehrlich.[37] In the author's opinion, this is misleading. Ehrlich's argument (with which the author agrees) is that, in the above notation, variations of $V_m(x,y)$ over the surface are small compared to V_m itself. This does not seem directly relevant. A more relevant criterion would seem to be the smoothness of the surface which contains the points of closest approach to the solid of the incident gas atoms, assum-

ing for simplicity that they have equal energy E. Assuming, again for simplicity, that the lattice is not disturbed by the interaction, this surface is defined by $z=z_E(\mathrm{FL},x,y,r_0/a,\epsilon)$, where

$$V(\mathrm{FL},x,y,z_E,r_0/a,\epsilon)=E. \qquad (6)$$

For each case, effective interaction radii R_E for the energy E may be defined as those radii of spherical lattice atoms which result in surfaces giving best fits (in a sense defined below) to the variations of $z=z_E(\mathrm{FL},x,y,r_0/a,\epsilon)$ with x and y. An *upper limit* on the smoothness of the surface (that is, on R_E) is provided by setting $E=0$; that is, all incident gas atoms must penetrate at least to the surface $z=z_0$ (without the above assumption of an undisturbed lattice, some atoms need not penetrate this far, but these are trapped).

In the theory of gas-surface interactions, it is necessary[38] to know the "average" potential well, denoted by $-\bar{V}_m(\mathrm{FL},r_0/a,\epsilon)$, encountered by a gas atom during its approach to the surface. Later on, more detailed information will be required by the theory; for example, it will be necessary to know $V_m(\mathrm{FL},x,y,r_0/a,\epsilon)$ as a function of x and y.

II. LATTICE SUMS

Because of the considerations in the previous three paragraphs, we are interested in details of the variation of the gas-surface interaction energy V with z at several positions on each lattice face. Lattice sums calculated

Fig. 1. The 110b (a), f (b), and s (c) faces. The filled circles represent solid atoms at $z/a=-2^{\frac{1}{2}}n$ for b and s and at $z/a=-n/2^{\frac{1}{2}}$ for f where $n=0,1,2,\cdots,\infty$; the open circles represent solid atoms at $z/a=-2^{\frac{1}{2}}(n+\frac{1}{2})$ for b and s and at $z/a=-(n+\frac{1}{2})/2^{\frac{1}{2}}$ for f. The crosses for b and f give the positions (x,y) at which the gas-solid interaction potentials are calculated; for s they give the positions for the lattice sums.
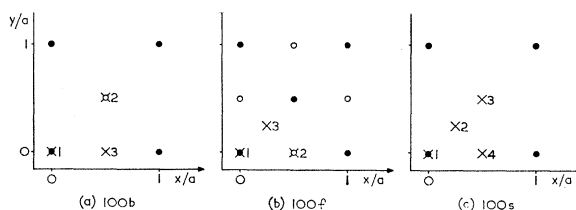
Fig. 2. The 100b (a), f (b), and s (c) faces. The filled circles represent solid atoms at $z/a=-n$ and the open circles solid atoms at $z/a=-(n+\frac{1}{2})$ where $n=0,1,2,\cdots,\infty$. The crosses for b and f give the positions (x,y) at which the gas-solid interaction potentials are calculated; for s they give the positions for the lattice sums.

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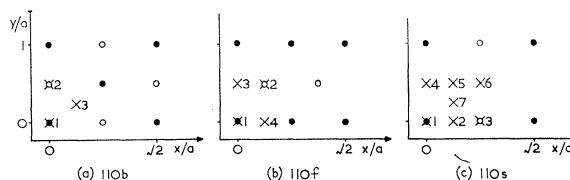[37] G. Ehrlich, Ann. Acad. Sci. (N. Y.) **101**, 722 (1963).

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TABLE I. Coordinates of the surface positions (Refs. 24, 25), in Figs. 1 and 2, at which the interaction potentials are calculated as functions of z.

110LN	$4x/2^{\frac{1}{2}}a$	$4y/a$	100LN	$4x/a$	$4y/a$
s1	0	0	s1	0	0
s2	1	0	s2	1	1
s3	2	0	s3	2	2
s4	0	2	s4	2	0
s5	1	2	b1	0	0
s6	2	2	b2	2	2
s7	1	1	b3	2	0
b1	0	0	f1	0	0
b2	0	2	f2	2	0
b3	1	1	f3	1	1
f1	0	0			
f2	1	2			
f3	0	2			
f4	1	0			

as functions of z at each of the seven positions marked on the 110s face in Fig. 1(c) enable V to be evaluated as a function of z at the three positions on the 110b face in Fig. 1(a) and at the four on the 110f in Fig. 1(b). Similarly, sums calculated as functions of z at each of the four positions marked on the 100s face in Fig. 2(c) enable V to be evaluated as a function of z at the three positions on each of the 100b and 100f in Figs. 2(a) and 2(b), respectively. Position N on the FL face is denoted by FLN; for example, $V(100b,a/2,0,z,r_0/a,\epsilon)$ is equivalent to $V(100b3,z,r_0/a,\epsilon)$. Absolute clarity as to the coordinates of each position is essential; for this reason they are given, relative to the axes in Figs. 1 and 2, in Table I.

For the 110s face, the sums are done at $32z/2^{\frac{1}{2}}a=0(1)56$ for each position, and for the 100s at $20z/a=0(1)50$. Then, $V(110L N,z,r_0/a,\epsilon)$ may be calculated at $32z/2^{\frac{1}{2}}a=0(1)48$ and $V(100L N,z,r_0/a,\epsilon)$ at $20z/a=0(1)40$; the calculations are done for $r_0/a=0.6(0.1)2$. For each case z_0 and z_m are each found by approximating $V(z)$ by a Lagrangian seven-point interpolation polynomial,[39] the central point being chosen as that closest to z_0 or z_m [z_0 and z_m are, respectively, the finite roots of $V(z)=0$ and $dV(z)/dz=0$, found by Newton's method from the interpolation polynomials].

Position 2 is the adsorption site for all the b and f cases considered, and the easiest route of surface diffusion is via position 3. Thus we assume that

$$H(\mathrm{FL},r_0/a,\epsilon)=-V_m(\mathrm{FL}2,r_0/a,\epsilon) \qquad (7)$$

and

$$D(\mathrm{FL},r_0/a,\epsilon)=V_m(\mathrm{FL}3,r_0/a,\epsilon)-V_m(\mathrm{FL}2,r_0/a,\epsilon). \qquad (8)$$

The effective radius $R_0(\mathrm{FL}1N,r_0/a)$ for zero energy and for the pair of points 1,N ($N=2,3,4$) is defined as that radius of spherical lattice atoms which results in a difference in surface height between the points 1 and N equal to the difference between $z_0(\mathrm{FL}1,r_0/a)$ and $z_0(\mathrm{FL}N,r_0/a)$. Denoting this difference by $\Delta z_0(\mathrm{FL}1N,r_0/a)$, we obtain

in general

$$32R_0(\mathrm{FL}1N,r_0/a)$$
$$=16\Delta z_0(\mathrm{FL}1N,r_0/a)+ca^2/\Delta z(\mathrm{FL}1N,r_0/a), \qquad (9)$$

where $c=4$, 3, 6, 4, 2, 8, 4, 4, and 2, respectively, for FL$1N=$110b12, 110b13, 110f12, 110f13, 110f14, 100b12, 100b13, 100f12, and 100f13. If $z_0(110f2,r_0/a)<2^{\frac{1}{2}}a/4$, then (9) does not hold for $R_0(100f12,r_0/a)$ because then the energy zero over position 2 is nearer to the lattice atom immediately below it in the second layer [at the point $(a/8^{\frac{1}{2}},a/2,-a/8^{\frac{1}{2}})$] than to that in the first layer at position 1 (at the origin). In this case we take

$$2R_0(110f12,r_0/a)$$
$$=z_0(110f1,r_0/a)+z_0(110f2,r_0/a)+1/8^{\frac{1}{2}}. \qquad (10)$$

The average potential well $-\bar{V}_m(\mathrm{FL})$ is calculated in each case from $V_m(\mathrm{FL}N)$ by assuming that V_m varies sinusoidally with x and y. That is, we assume that

$$4\bar{V}_m(\mathrm{FL})=V_m(\mathrm{FL}1)+V_m(\mathrm{FL}2)+2V_m(\mathrm{FL}3) \qquad (11a)$$

for FL$=$100b, 100f and 110b, and that

$$4\bar{V}_m(\mathrm{FL})=V_m(\mathrm{FL}1)+V_m(\mathrm{FL}2)$$
$$+V_m(\mathrm{FL}3)+V_m(\mathrm{FL}4) \qquad (11b)$$

for FL$=$110f.

III. PREVIOUS WORK

The first semi-infinite lattice sums of which the author is aware are those of Orr,[40] who tabulated $S_6(100sN,z)$ for combinations of $N=1$, 3 and 4 and $8z=0$, 4, 5, 8, 12, and 16. For each of these three positions, an analytic expression was devised to give a reasonable fit of $V(z)$. Orr's tables were later supplemented by those of Steele and Halsey[41] on $S_{12}(100sN,z)$. The interaction of gases with a semi-infinite graphite crystal was considered by Crowell[42,43] and by Crowell and Steele.[44] The most accurate published calculations available to date appear to be those of Steele and Ross,[45] who tabulated $S_k(100s,x,y,z)$ for combinations of $k=6$ and 12, all our positions 1–4 [Fig. 2(c)] as well as $(8x/a,8y/a)=(1,1)$, (3,3), (4,3), (2,0), (3,1), and (4,2), and $20z/a=0(1)25$ and 26(2)50 [for our position 3 calculations were done also for $20z/a=50(2)80$]. These sums enabled evaluation of the gas-surface interaction energy at the six positions (our three and three others) on the 100f face shown in Fig. 3 of Ref. 46. Results for V_m at each position were applied successfully[46,47] to the special case of the adsorption of He on Ar. The lattice

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sums were tabulated to four or five significant figures, and the accuracy is as expected[45] by the authors: For the smallest values of z, five significant figures are correct for S_{12}, and usually for S_6; for the largest values of z, four figures are correct for S_{12}, but only two for S_6.

The b lattice was considered in some detail by Neustadter and Bacigalupi,[48] who calculated the interaction energy at up to one hundred and thirty-two positions on each of the eight surface planes of highest atom density, for four specific values of r_0/a. Their resulting values of H/ϵ and D/ϵ are tabulated and topographical potential maps drawn; the comparison with experimental data seems encouraging. Results obtained in this paper are essentially in agreement with those of Bacigalupi and Neustadter[48] where direct comparison is possible. However, the accuracy of their sums is stated by the authors to be only about 1%.

Other work in which semi-infinite lattice sums have been done is that of Oman's group,[30-33] referred to above. In this work, detailed gas-atom trajectories are calculated by integration of the classical equations of motion. However, the sums are incidental to the trajectory calculations and are not a main objective.

IV. PRESENT WORK

The calculations presented here are somewhat time consuming, but seem worthwhile as they find use in many related fields. For example, the 110s sums are a first step towards a calculation of the adsorption properties of He on the 110 face of Ar, complementary to the work of Ross and Steele[46,47] on the 100 Ar face; a comparison of these properties would be interesting, although this may involve further 110s sums, as the surface potential on the 110f face may be required at more than four positions (Ross and Steele[46] used six positions on the simpler 100f face). For these reasons, the results of the 110s and 100s sums are tabulated, respectively, in Appendices B and C, correct to five significant figures [except for a small chance of an error of ± 1 in the last figure for S_6(110s); see Appendix B]. The method of calculation is described in these Appendices.

In presentation of final results of the analysis (Figs. 3–11) in dimensionless form, energies are reduced by ϵ and lengths by d, defined by

$$d^3 = v. \tag{12}$$

(v is the lattice atomic volume). d is chosen rather than the more conventional a for the following reason. The heat of adsorption H is mainly determined by interaction of the gas atom with large, far-removed, portions of the lattice. Hence H/ϵ should be determined essentially by the average number, proportional to $(r_0/d)^3$, of solid atoms in a sphere of radius r_0. It is to be ex

[48] H. E. Neustadter and R. J. Bacigalupi, Surface Sci. 6, 246 (1967).
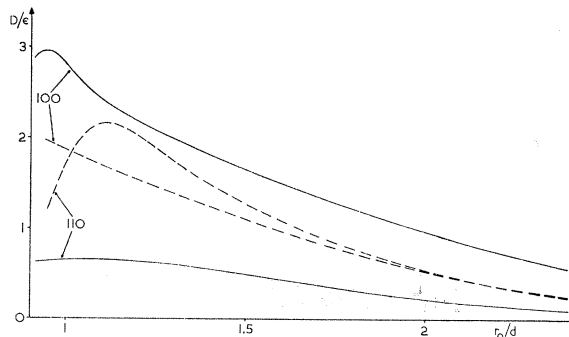
FIG. 3. $D(b)/\epsilon$ (———) and $D(f)/\epsilon$ (– – – –) versus r_0/d for the 110 and 100 faces.
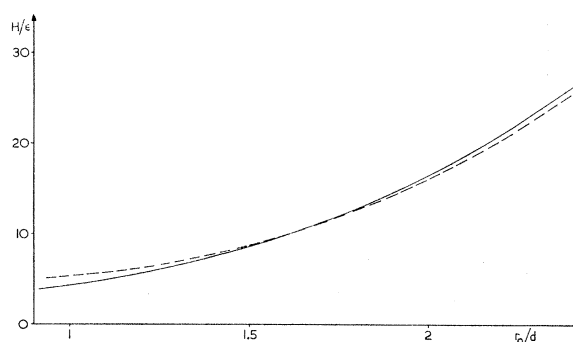
FIG. 4. $H(110b)/\epsilon$ (———) and $H(100f)/\epsilon$ (– – – –) versus r_0/d.
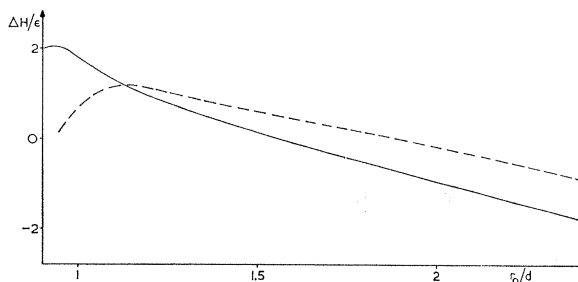
FIG. 5. $[H(100b)-H(110b)]/\epsilon$ (———) and $[H(110f)-H(100f)]/\epsilon$ (– – – –) versus r_0/d.
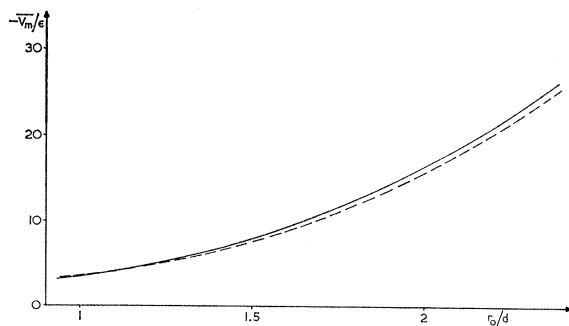
FIG. 6. $-\bar{V}_m(110b)/\epsilon$ (———) and $-\bar{V}_m(100f)/\epsilon$ (– – – –) versus r_0/d.

pected, therefore, that curves of H/ϵ versus r_0/d should, very approximately, be about the same for all lattice faces, especially for large r_0/d. This similarity may not
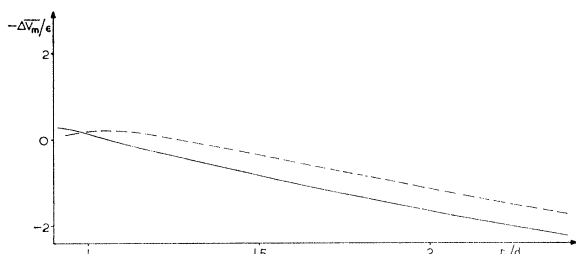
FIG. 7. $-[\bar{V}_m(100\text{b})-\bar{V}_m(110\text{b})]/\epsilon$ (———) and
$-[\bar{V}_m(110\text{f})-\bar{V}_m(100\text{f})]/\epsilon$ (- - - -) versus r_0/d.
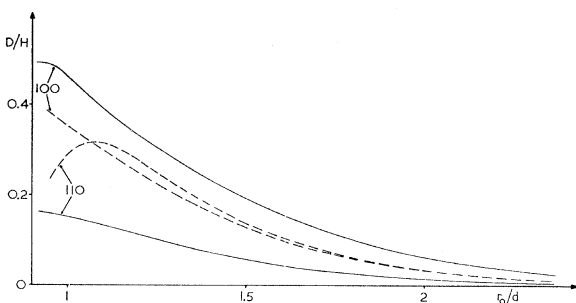
FIG. 8. $D(\text{b})/H(\text{b})$ (———) and $D(\text{f})/H(\text{f})$ (- - - -)
versus r_0/d for the 110 and 100 faces.
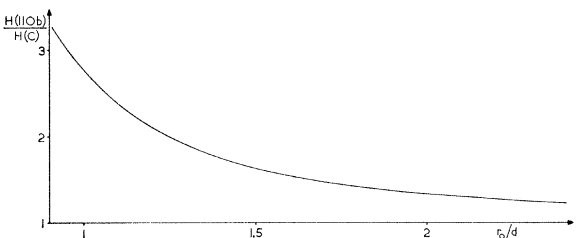
FIG. 9. $H(110\text{b})/H(\text{C})$ versus r_0/d.
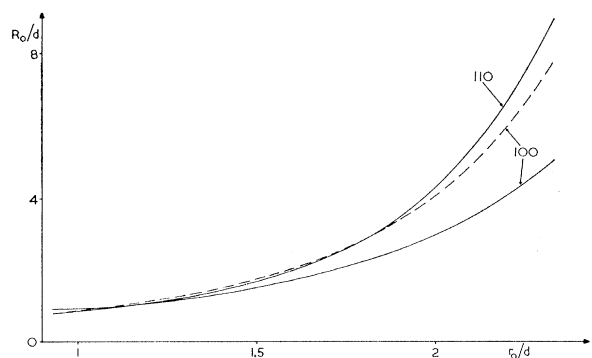
FIG. 10. $R_0(110\text{b}12)/d$ and $R_0(100\text{b}12)/d$ (———)
and $R_0(100\text{f}12)/d$ (- - - -) versus r_0/d.

be clear from curves of H/ϵ versus r_0/a, as the relation
between d and a depends on the lattice type; for
example,

$$(a/d)^3 = 2(\text{b}); \quad 4(\text{f}). \tag{13}$$

The same arguments apply to the average potential
well $-\bar{V}_m$, discussed above. These arguments do not,
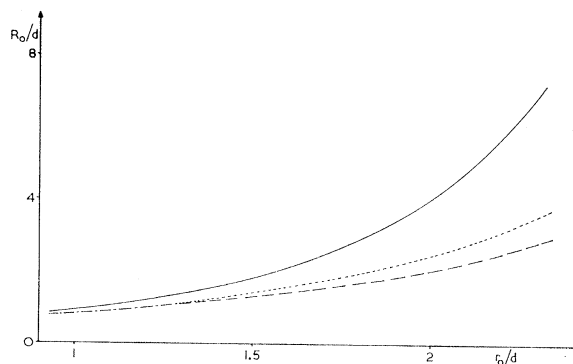

FIG. 11. $R_0(110\text{f}1N)/d$ versus r_0/d for $N=2$ ($\cdots\cdots$),
$N=3$ (- - - -), and $N=4$ (———).

however, apply to the heat of surface diffusion D, which
is mainly determined by interaction of the gas atom
with the nearest portions of the lattice. Curves of D/ϵ
versus r_0/d are, therefore, expected to depend strongly
on the lattice face under consideration, especially for
small r_0/d; similar statements apply to curves of R_0/d
and of D/H versus r_0/d. However, as $r_0/d \to \infty$, even
the nearest portions of the lattice become far-removed,
and the results on all lattice faces approach those ob-
tained from a continuum model of the solid. The
continuum "face" is denoted by FL$=$C, and the
corresponding results are as follows:

$$\frac{H(\text{C})}{\epsilon} = -\frac{V_m(\text{C})}{\epsilon} = \frac{20^{\frac{1}{2}}\pi}{9}\left(\frac{r_0}{d}\right)^3, \tag{14}$$

$$D(\text{C})/\epsilon = 0, \quad R_0(\text{C})/d = \infty. \tag{15}$$

Figure 3 contains the results for D/ϵ on the four
lattice faces considered. The curves of H/ϵ are about
the same for all four faces (see above); to avoid con-
fusion, therefore, the results for the 110b and 100f faces
(that of higher surface-atom density in each case) are
given in Fig. 4, and the differences between these results
and those for the 100b and 110f faces, respectively, in
Fig. 5. In the same way, the curves of $-\bar{V}_m/\epsilon$ for the
110b and 100f faces are given in Fig. 6, and the differ-
ences between these and those for the 100b and 110f
faces, respectively, in Fig. 7. (Remember that $V_m<0$
always.) Curves of D/H are important (see below),
and these are shown for the four faces in Fig. 8.

It is instructive to compare the lattice results on H
and $\bar{V}_m$ with those (14) from the continuum solid model.
As all the curves of H and $-\bar{V}_m$ are similar (see Figs. 4–
7), this comparison is made by plotting $H(110\text{b})/H(\text{C})$
versus r_0/d in Fig. 9.

For each of FL$=$110b, 100b and 100f, $R_0(\text{FL}12)$ is
close the corresponding $R_0(\text{FL}13)$ for the same value
of r_0; for these three faces, therefore, only $R_0(\text{FL}12)$ is
shown versus r_0 in Fig. 10. In contrast, the values of
$R_0(110\text{f}1N)$ for $N=2$, 3, and 4 are *not* close; for ex-
ample, $N=4$ gives markedly higher results than either

TABLE II. Theoretical results for self-interaction (Refs. 24, 25).

FL	r_0/d	λ/ϵ	H/ϵ	D/ϵ	D/H	H/λ	D/λ
110b	1.146	8.245	5.23	0.64	0.123	0.634	0.078
100b	1.146	8.245	6.35	2.30	0.362	0.770	0.279
110f	1.156	8.610	7.14	2.12	0.297	0.829	0.246
100f	1.156	8.610	5.96	1.61	0.270	0.692	0.187

TABLE III. Summary of experimental data on self-interaction, and some theoretical results.

System	D (kcal/mole)	λ[a] (kcal/mole)	D/λ (experimental)	r_0[b] (A)	ϵ[c] (kcal/mole)
Au	23[d,e]	90.7	0.25[f,e]	2.96	10.5
K	0.5[g,e]	21.8	0.02[h,e]	4.85	2.64
W(110)	22[i]	204	0.11[j]	2.88	24.7

[a] Quoted in Ref. 8.
[b] From Eq. (2a) and C. Kittel, *Introduction to Solid State Physics* (John Wiley & Sons, Inc., New York, 1963), p. 40.
[c] From Eq. (2b) and column 3.
[d] A. J. Melmed and R. Gomer, J. Chem. Phys. **34**, 1802 (1961).
[e] It is doubtful whether the methods used to obtain these data are valid; see J. A. Simmons *et al.*, J. Appl. Phys. **35**, 2271 (1964); V. Ruth and J. P. Hirth, J. Chem. Phys. **41**, 3139 (1964).
[f] In agreement with theoretical 110 value in Table II; see footnote e, however.
[g] R. L. Parker and S. C. Hardy, J. Chem. Phys. **37**, 1606 (1962).
[h] An unrealistically low value (footnote g); see footnote e.
[i] Reference 57.
[j] Somewhat larger than the theoretical result 0.08 in Table II.

$N=2$ or $N=3$, particularly at the larger r_0. For this reason, all three curves of R_0 for the 110f face are shown in Fig. 11.

In many ways, the simplest example of "gas-solid" interaction is that of "self-interaction" (that is, the interaction of an atom with its own lattice), for which r_0/d is calculated from (2a) and (13), and H/ϵ, D/ϵ, and D/H then follow from Figs. 3–5 and 8. Also of considerable interest are λ/ϵ, H/λ, and D/λ, where λ/ϵ is the reduced heat of sublimation, calculated from (2b). (It is as well to emphasize here that the heat of sublimation is *not* the same as, but is greater than, the heat of self-adsorption at "zero coverage".) These results for self-interaction are in Table II. (Note that our value 1.146 of r_0/d for the b lattice differs from that, 1.112, which corresponds to the $\sigma/a_0 = 0.786$ of Neustadter and Bacigalupi.[48])

V. COMPARISON WITH EXPERIMENT AND DISCUSSION

For self-interaction, r_0/d is fixed as described in the previous paragraph, whereas, for other gas-solid systems, it must be estimated, either by comparison of our results with experiment or by some independent means. Perhaps the best method is from experimental values of H/D on a known crystal face; in general, H/D determines r_0/d from Fig. 8. An independent method involves using the well-known combination rule in conjunction with values of r_0 for the gas-gas and solid-solid systems (see, for example, Ref. 49).

In most cases, the crystal faces predominating during the experiments are unknown. For example, estimates of the main faces to be expected on an etched W filament vary from mainly 100 with a possibility of some 110 (Ref. 50) through a mixture of 110 and 211 (Ref. 51) to mainly 110 (see Refs. 48, 52, 53). This information is important for an adequate comparison of theory with experiment, as, for given L, D/ϵ is very dependent on F, although H/ϵ is not so dependent (see Figs. 3–5). Where this information is lacking, however, it *may* be possible to make certain statements about F from a comparison with the theory; for example, it is impossible (see Fig. 8) to obtain $D/H > 0.32$ for any gas on a 110f surface.

For cases in which there are no reliable independent

estimates of r_0 for the gas-gas systems, results for many gases on the same surface are not sufficient in general; a satisfactory test of the theory is obtained in general only if experimental results are available for the same gas on more than one surface (preferably of the same solid). This is because r_0 for solids is easily estimated from (2a), and when r_0 for one gas-solid system is known (by comparison with the theory, for example), the combination rule allows estimation of r_0 for the interaction of the *same* gas with another solid; of course, r_0 should be independent of which surface of the *same* solid is considered.

Table III contains a summary of experimental data on the self-interaction of Au, K, and W, although it seems that little reliance may be placed on the data for Au and K (see footnote e); theoretical values of r_0 and ϵ are included to illustrate expected values. A summary of experimental data and corresponding theoretical results on "mixed" systems is given in Table IV. The agreement between the experimental data on D/H for O-W and N-W and the theoretical values for $F=100$ does not constitute a satisfactory test of the theory, except for the fact that "reasonable" values of r_0 are obtained for these systems (for a 100 face). Similar remarks apply to K-W, where the experimental result falls between the theoretical 110 and 100 values. On the other hand, r_0 for H-W is calculated from that for H-Ni, and the agreement here is more encouraging. Similarly, the agreement for Ba-W (100 and 110) is quite satisfactory, as r_0 for these systems is calculated independently. Because the Cs atom is so large ($a \simeq 6A$), the pairwise model predicts values of D/H for Cs-W considerably lower than the experimental result, which is very discouraging. Worse is the situation for the inert gas-W systems, where it may reasonably be assumed that the pairwise model should be relatively good. The fact that D/H is larger for Xe-W than for Ar-W is contrary to the predictions of the model, as it is almost certain that r_0 for Xe-W would be larger than for Ar-W (considerable weight is given to this remark by the re-

[49] F. O. Goodman, J. Phys. Chem. Solids **24**, 1451 (1963).
[50] R. P. Johnson, Phys. Rev. **54**, 459 (1938).
[51] R. P. Bien, Phys. Rev. **47**, 806 (1935).
[52] I. Langmuir, J. Am. Chem. Soc. **54**, 2798 (1932).
[53] F. L. Hughes *et al.*, Phys. Rev. **113**, 1023 (1959).

TABLE IV. Summary of experimental data on mixed systems, and some theoretical results.

System	r_0/d	D/H (theory)[a] F=110	D/H (theory)[a] F=100	D/H (experiment)	r_0^b (A)	ε (kcal/mole)
Ba-W(110)		0.060		0.06d		9.8e
	1.48c				3.8	
Ba-W(100)			0.20	0.17d		
K-W	1.54c	0.051	0.18	0.11f	3.9	6.9g
Cs-W	1.67c	0.035	0.13	0.22d		
Ar-W	1.34h	0.083	0.26	0.32d		i
Kr-W	1.38h	0.076	0.24	>0.25d		
Xe-W	1.48h	0.060	0.20	0.42d		
H-Ni	1.57j	0.11	0.11	0.11d	3.5	6.6e
H-W	1.45k	0.064	0.21	0.22d	3.6	9.1l
O-W	1.47m	0.061	0.20	0.20d	3.7	17l
N-W	1.40m	0.072	0.23	0.23n	3.5	19l

a From Fig. 8 and column 2.
b From column 2.
c From the combination rule (Ref. 49) used on values of r_0 for Ba, K, Cs, and W (4.56A, 4.85A, 5.50A, and 2.88A, respectively) obtained by combining Eq. (2a) with values of a in C. Kittel, *Introduction to Solid State Physics* (John Wiley & Sons, Inc., New York, 1963), p. 40.
d Quoted in G. Ehrlich, General Electric Research Laboratory Report No. 59-RL-2299M, 1959 (unpublished). (Note that $D/H \approx 0.20$ for O-W).
e Average values obtained by comparison of the experimental D and H quoted in footnote d with the corresponding theoretical D/ϵ and H/ϵ curves in Figs. 3–5, using the r_0/d in column 2.
f L. Schmidt and R. Gomer, J. Chem. Phys. 42, 3573 (1965).
g As in footnote e, but adding 54% of the 110 results to 46% of the 100.
h From the combination rule used on values of r_0 for Ar, Kr, and Xe in Ref. 49 and r_0 for W in footnote c.
i Agreement of theory with experiment is so poor (see Sec. V) that further calculations are unjustified.
j From comparison of the experimental D/H in column 5 with the corresponding theoretical curves in Fig. 8.
k From the combination rule used on values of r_0 for W and Ni (2.56A for Ni) from footnote c and r_0/d for H-Ni in this table.
l As in footnote e, but assuming a 100 surface.
m Obtained by the method of footnote j, but assuming a 100 surface.
n Quoted in Ref. 37.

sults of Ref. 54). The experimental value[55] of D for Xe-W was, in fact, for the 310 face. From the pairwise theory,[48] $D(100)>D(310)$, which makes the agreement even worse. For a reasonable value of r_0/d, the theory cannot reproduce the experimental result $D/H=0.42$ on any of the eight faces studied in Ref. 48 (the largest value $\simeq 0.32$ for the 411). One may hope that this relatively large D/H is incorrect, but this is unlikely as it would need reduction by a factor of about 2 to conform to pairwise theory.

VI. FURTHER DISCUSSION

The above comparisons of theory with experiment are discouraging, and no decision can be made at present as to circumstances in which the pairwise model is appropriate for calculations of gas-solid interaction, except perhaps for inert-gas–inert-gas solid systems, for which it may be expected to work well. It is felt, however, that the model may at least be useful in some approximate sense, for example for order-of-magnitude calculations. A summary of points against and for the model is found in Appendix A.

With the above reservations, let us estimate values of effective interaction radii R_0 for zero energy (see Sec. I) to be expected in gas-surface scattering experiments. From Table IV, for gas-W systems, r_0/d lies in the range 1.3–1.5, and from Fig. 10, R_0/d lies in the range 1.2–1.7 (for 100 and 110 surfaces). The hard-spheres radii R in Ref. 29 correspond to $R_0/d \simeq 1.3$, 1.4, and 1.5, respec-

54 F. O. Goodman, Ref. 31, p. 366.
55 G. Ehrlich and F. G. Hudda, J. Chem. Phys. 30, 493 (1959).

tively, for He, Ar, and Xe-W, and the W surfaces actually "seen" by the gas atoms are, therefore, about as "rough" as those in Ref. 29, and can certainly not be called "smooth."[56] We conclude, then, that although the success[26,27] of the hard-cubes theory in describing experimental gas-surface scattering patterns is a point against the pairwise theory (Appendix A), the smooth-surface assumption is not justified by experimental adsorption and surface-diffusion data.

From the results on the relative magnitudes of $R_0(FL1N)$, stated in Sec. IV and illustrated in Figs. 10 and 11, it seems that gas-surface scattering properties should not depend strongly on incident azimuth angle (ϕ_0 of Refs. 28 and 29) for the 110b, 100b, or 100f faces, but that this dependence may be strong for the 110f. This is in agreement with previous conclusions.[28,29,32,33]

It is argued in Sec. IV that curves of H/ϵ versus r_0/d should be approximately the same for all lattice faces, because H/ϵ is determined mainly by long-distance atom-atom interactions, and this is supported by Figs. 4 and 5. In spite of this, the comparison made in Fig. 9 of H(110b) with the continuum result H(C), makes it clear that *some* short-range effects *are* important, particularly for small r_0/d. It follows that considerable care must be taken using a continuum model of adsorption, as this may underestimate H/ϵ by as much as 40–50% in the region of interest. The asymptotic result H(FL)=H(C) does not appear to be even approximately true unless r_0/d is very large. This result echoes similar conclusions of Steele and Ross.[45]

Figures 6 and 7 provide a firm basis for estimation of $\bar{V}_m$, a quantity important in gas-surface interaction theory. In the region of interest, $-\bar{V}_m/\epsilon \simeq 5$–8, whereas values of $H/\epsilon \simeq 6$–9 are, of course, slightly larger.

VII. CONCLUSIONS

Some of the present experimental data on surface-diffusion and adsorption properties are inconsistent with the pairwise theory, while others support it; over all, however, there seems to be a general inconsistency of the data with the theory. These data are not inconsistent with the hard-cubes theory, but can offer it no support because they give information about parts of the gas-surface interaction potential which are not directly relevant to the hard-cubes model. The pairwise theory is inconsistent with the hard-cubes theory.

The present data are rather sparse and, perhaps, some are unreliable, so it is too early to suggest rejection of the pairwise theory. There is, therefore, considerable need for a series of reliable experimental data on several suitably chosen gas-surface systems, for example the inert gases on several faces of as many f and b metals as possible.

If, as seems likely at present, it eventually turns out that the pairwise model must be rejected, then a new

56 In fact, on the basis of these arguments it seems that these (Ref. 29) values of R are slightly too large.

interaction model must be constructed which will be either consistent or inconsistent with the hard-cubes theory, which theory may by then have been either accepted or rejected on other grounds.

On the other hand, if it turns out that the data are consistent with the pairwise model, then, presumably, this model will be either accepted, in which case the hard-cubes theory will be rejected, or rejected in favor of a new interaction model which is consistent with both the hard-cubes theory (in the region of the interaction potential relevant to gas-surface scattering) and the pairwise theory (in the region relevant to adsorption and surface diffusion).

ACKNOWLEDGMENTS

APPENDIX A: SUMMARY OF POINTS AGAINST AND FOR THE PAIRWISE MODEL OF GAS-SURFACE INTERACTIONS

Against

(1) The experimental and theoretical Cs-W results disagree.

(2) The qualitative experimental behavior of D/H for the inert gas-W systems is contrary to that of the theory.

(3) From comparison of experimental and theoretical results on the relative values of D for self-interaction of W-W on five different faces, Ehrlich and Hudda[57] conclude that the model is inadequate for the W-W surface interactions.

(4) The smooth-surface (hard-cubes) theory of gas-surface scattering is successful[26,27] (see Sec. VI).

For

(1) All values of r_0 in Table IV are reasonable. The Ba-W (110 and 100) results are consistent, as are results for H-Ni and H-W with the assumption of a 100 surface for W and a combination of 110 and 100 for Ni.

(2) Neustadter and Bacigalupi[48] conclude that their comparison with experiment gives considerable support to the pairwise model, particularly for inert gas-metal systems. However, these conclusions should, perhaps,

be modified in view of the conclusions here and in Ref. 57.

(3) Some justification is afforded (at least on the 100b face) for the empirical result[37] $D/H \simeq 0.2$, as this result obtains in the region of "realistic" r_0/d for many systems (see Fig. 8 and Table IV).

(4) Results of Refs. 46 and 47 on He-Ar suggest that the model may be valid for inert-gas–inert-gas solid systems. It is well known that the model works well for inert-gas–inert-gas systems, and for a description of properties of inert gas solids, so this result is not surprising.

(5) Lattice theories of thermal accommodation coefficients, in which pairwise potentials are used, work well.[49,54] However, this is by no means a rigorous test of the pairwise model because only "head-on" interaction of the gas atom with only one surface atom is considered, and because the thermal accommodation coefficient gives a very "coarse-grained" picture of the scattering process.

APPENDIX B: RESULTS OF THE 110s LATTICE SUMS

In Table V we present the results of the lattice sums on the 110s face at each of the seven positions in Fig. 1(c) as functions of the distance z of the gas atom from the surface; the coordinates, relative to the axes in Fig. 1(c), of each position are in Table I.

The sums are calculated by direct summation over the lattice atoms for gas-atom–solid-atom distances less than some distance l, which depends on z; the contribution to the summation from lattice atoms more remote than l is approximated by an integral. The criterion for the choice of l is that five significant figures may be obtained for S_6; this results in about ten significant figures for S_{12}. The complete range of z is separated into five smaller ranges by the four values of $32z/2^{\frac{1}{2}}a = 11$, 22, 33, and 45, each of these being a maximum of one of the smaller ranges. In each range, the results obtained using some initial, arbitrarily chosen value l_0 of l are compared with those obtained using a much larger value l_1 for one or two values of z; this process is repeated with different choices of l_0 and l_1 until a sufficiently large l_0 is found, together with an appropriate correction (obtained from the much larger l_1). With this procedure, the values of l_0 finally chosen for the five ranges are $l_0/a = 10$, 12, 20, 26, and 36, respectively; the larger values of l_1 depend on the particular case considered, but in general $l_1/a = 16$, 24, 40, 50, and 60, respectively. Finally, all results are rounded to five significant figures. All figures quoted for S_{12} are correct, while there is a small chance of an error of ± 1 in the last figure for S_6; this error in S_6 should occur, if at all, in very few cases, as any clearly doubtful case is recalculated using larger and larger l.

As stated in Sec. II, z_0 and z_m are each calculated by approximating $V(z)$ by a Lagrangian seven-point inter-

[57] G. Ehrlich and F. G. Hudda, J. Chem. Phys. 44, 1039 (1966).

TABLE V. Results of the sums for the (110) simple cubic lattice face.

$32z/z^2a$	$S_6(110s1,z)$	$S_{12}(110s1,z)$	$S_6(110s2,z)$	$S_{12}(110s2,z)$	$S_6(110s3,z)$	$S_{12}(110s3,z)$	$S_6(110s4,z)$	$S_{12}(110s4,z)$	$S_6(110s5,z)$	$S_{12}(110s5,z)$	$S_6(110s6,z)$	$S_{12}(110s6,z)$	$S_6(110s7,z)$	$S_{12}(110s7,z)$
-1	1.3422(8)	∞	5.1982(2)	2.6216(5)	2.6519(1)	1.9255(2)	1.2864(2)	7.8198(3)	4.2846(1)	7.2402(2)	1.6546(1)	4.0786(1)	1.6057(2)	2.3034(4)
-0	2.0972(6)	1.8014(16)	4.9537	2.3887	2.3767	1.5646	1.3121	8.1931	4.1606	7.0039	1.5197	3.3746	1.5500	2.1642
0	1.8412(5)	4.3980(12)	4.3260	1.8221	2.1488	1.3266	1.2792	7.8191	3.9378	6.3775	1.4028	2.9009	1.4138	1.8027
1	3.2772(4)	3.3897(10)	3.5005	1.1904	1.9426	1.1259	1.1929	6.8116	3.6335	5.4793	1.2963	2.5371	1.2242	1.3453
2	2.8800	1.0737(9)	2.6660	6.8723(4)	1.7466	9.3750(1)	1.0672	5.4496	3.2733	4.4604	1.1957	2.2216	1.0140	9.1356(3)
3	1.1438	7.3787(7)	1.9437	3.6250	1.5575	7.5979	9.1991(1)	4.0412	2.8855	3.4589	1.0982	1.9276	8.1072(1)	5.7474
4	5.1473(2)	8.2757(6)	1.3779	1.8016	1.3762	5.9836	7.6840	2.8520	2.4961	2.5710	1.0030	1.6474	6.3147	3.4116
5	2.5504	1.3015	9.6241(1)	8.6540(3)	1.2051	4.5855	6.2571	1.8520	2.1254	1.8436	9.1027(0)	1.3830	4.8336	1.9432
6	1.3647	2.6215(5)	6.6908	4.0971	1.0468	3.4292	4.9965	7.1192(2)	1.7872	1.2837	8.2061	1.1396	3.6663	1.0777
7	7.7807(1)	6.3785(4)	4.6653	1.9391	9.0297(0)	2.5112	3.9343	4.3239	1.4884	8.7325(1)	7.3500	9.2218(0)	2.7659	5.8896(2)
8	4.6799	1.8015	3.2802	9.2659(2)	7.7470	1.8073	3.0696	2.5655	1.2312	5.8338	6.5434	7.3372	2.0905	3.2016
9	2.0209	5.7406(3)	2.3342	4.4992	6.6199	1.2828	2.3830	1.5123	1.0141	3.8504	5.7939	5.7492	1.5874	1.7438
10	2.9478	2.0209	1.6850	2.2291	5.6419	9.0093(0)	1.8469	8.9022(1)	8.3357(0)	2.5190	5.1061	4.4446	1.2140	9.5665(1)
11	1.9333	7.7362(2)	1.2356	1.1295	4.8017	6.2795	1.4430	5.2537	6.8498	1.6400	4.4826	3.3965	9.3681(0)	5.3069
12	1.3142	3.1807	9.2097(0)	5.8608(1)	4.0854	4.3552	1.1156	3.1180	5.6358	1.0658	3.9231	2.5704	7.3013	2.9848
13	9.2239(0)	1.3909	6.9780	3.1153	3.4783	3.0126	8.7275(0)	1.8630	4.6484	6.9316(0)	3.4256	1.9298	5.7505	1.7051
14	6.6629	6.4197(1)	5.3727	1.6962	2.9656	2.0824	6.8703	1.1261	3.8472	4.5205	2.9865	1.4397	4.5775	9.9047(0)
15	4.9391	3.1073	4.2009	9.4565(0)	2.5336	1.4408	5.4470	6.8723(0)	3.1972	2.9609	2.6015	1.0690	3.6823	5.8536
16	3.7477	1.5692	3.3331	5.3950	2.1701	9.9929(-1)	4.3522	4.2416	2.6696	1.9504	2.2656	7.9098(-1)	2.9927	3.5204
17	2.9039	8.2322(0)	2.6810	3.1474	1.8642	6.9548	3.5058	2.6490	2.2402	1.2934	1.9738	5.8398	2.4561	2.1544
18	2.2929	4.4703	2.1840	1.8761	1.6065	4.8619	2.8477	1.6744	1.8898	8.6403(-1)	1.7209	4.3067	2.0346	1.3412
19	1.8413	2.5050	1.8001	1.1418	1.3892	3.4163	2.3327	1.0713	1.6029	5.8181	1.5023	3.1754	1.7002	8.4906(-1)
20	1.5012	1.4448	1.4996	7.0881(-1)	1.2054	2.4142	1.9269	6.9376(-1)	1.3668	3.9506	1.3136	2.3428	1.4326	5.4626
21	1.2406	8.5576(-1)	1.2616	4.4847	1.0497	1.7166	1.6047	4.5470	1.1718	2.7056	1.1507	1.7308	1.2164	3.5697
22	1.0378	5.1949	1.0709	2.8895	9.1745(-1)	1.2284	1.3470	3.0156	1.0099	1.8693	1.0102	1.2811	1.0402	2.3679
23	8.7756(-1)	3.2265	9.1640(-1)	1.8942	8.0472	8.8489(-2)	1.1395	2.0233	8.7487(-1)	1.3029	8.8894(-1)	9.5062(-2)	8.9554(-1)	1.5933
24	7.4930	2.0470	7.9006	1.2623	7.0835	6.4174	9.7094(-1)	1.3731	7.6166	9.1616(-2)	7.8418	7.0742	7.7581	1.0868
25	6.4538	1.3247	6.8576	8.5442(-2)	6.2570	4.6857	7.1960	9.4220(-2)	6.6627	6.4986	6.9356	5.2816	6.7599	7.5101(-2)
26	5.6023	8.7339(-2)	5.9893	5.8692	5.5458	3.4445	6.2542	6.5356	5.8551	4.6495	6.1506	3.9572	5.9221	5.2541
27	4.8974	5.8591	5.2607	4.0883	4.9319	2.5491	5.4676	4.5814	5.1680	3.3548	5.4693	2.9762	5.2143	3.7191
28	4.3086	3.9950	4.6450	2.8854	4.4040	1.8989	4.8061	3.2446	4.5807	2.4408	4.8769	2.2474	4.6128	2.6620
29	3.8124	2.7658	4.1210	2.0618	3.9381	1.4238	4.2464	2.3208	4.0764	1.7903	4.3607	1.7041	4.0987	1.9255
30	3.3911	1.9424	3.6724	1.4905	3.5353	1.0743	3.7699	1.6760	3.6414	1.3235	3.9097	1.2976	3.6569	1.4067
31	3.0308	1.3826	3.2862	1.0893	3.1831	8.1567(-3)	3.3619	1.2218	3.2645	9.8596(-3)	3.5149	9.9245(-3)	3.2753	1.0375
32	2.7206	9.6651(-3)	2.9519	8.0440(-3)	2.8741	6.2303	3.0107	8.9867(-3)	2.9367	7.3997	3.1684	7.6239	2.9443	7.7212(-3)
33	2.4519	7.2677	2.6610	5.9975	2.6022	4.7868	2.7067	6.6680	2.6504	5.5937	2.8635	5.8827	2.6557	5.7953
34	2.2180	5.3595	2.4068	4.5125	2.3622	3.6987	2.4423	4.9892	2.3993	4.2579	2.5946	4.5595	2.4031	4.3851
35	2.0132	3.9936	2.1837	3.4244	2.1498	2.8738	2.2113	3.7635	2.1785	3.2269	2.3567	3.5496	2.1811	3.3436
36	1.8332	3.0049	1.9872	2.6196	1.9613	2.2448	2.0086	2.8610	1.9834	2.5167	2.1459	2.7758	1.9853	2.5681
37	1.6741	2.2818	1.8133	2.0192	1.7935	1.7626	1.8299	2.1913	1.8106	1.9534	1.9584	2.1802	1.8119	1.9863
38	1.5331	1.7477	1.6589	1.5676	1.6437	1.3909	1.6718	1.6905	1.6570	1.5253	1.7914	1.7199	1.6580	1.5464
39	1.4075	1.3496	1.5214	1.2253	1.5098	1.1030	1.5315	1.3131	1.5201	1.1979	1.6423	1.3627	1.5207	1.2116
40	1.2954	1.0501	1.3986	9.6387(-4)	1.3896	8.7880(-4)	1.4064	1.0268	1.3976	9.4610(-4)	1.5087	1.0842	1.3981	9.5498(-4)
41	1.1949	8.2293(-4)	1.2885	7.6283	1.2816	7.0337	1.2946	8.0799(-4)	1.2878	7.5126	1.3889	8.6632(-4)	1.2882	7.5704
42	1.1045	6.4932	1.1896	6.0720	1.1843	5.6547	1.1943	6.3967	1.1891	5.9963	1.2811	6.9506	1.1893	6.0342
43	1.0231	5.1562	1.1004	4.8597	1.0963	4.5655	1.1041	5.0937	1.1001	4.8101	1.1839	5.5991	1.1003	4.8349
44	9.4944(-2)	4.1193	1.0199	3.9098	1.0167	3.7015	1.0228	4.0777	1.0197	3.8101	1.0960	4.5283	1.0198	3.8934
45	8.8270	3.3099	9.4698(-2)	3.1611	9.4452(-2)	3.0132	9.4924(-2)	3.2833	9.4680(-2)	3.1395	1.0165	3.6766	9.4689(-2)	3.1503
46	8.2206	2.6739	8.8079	2.5680	8.7888	2.4624	8.8255	2.6565	8.8066	2.5536	9.4437(-2)	2.9964	8.8072	2.5608
47	7.6684	2.1713	8.2057	2.0955	8.1909	2.0200	8.2196	2.1598	8.2048	2.0860	8.7877	2.4511	8.2053	2.0908
48	7.1644	1.7718	7.6568	1.7174	7.6453	1.6632	7.6677	1.7642	7.6562	1.7111	8.1901	2.0124	7.6565	1.7142
49	6.7036	1.4525	7.1555	1.4134	7.1445	1.3743	7.1639	1.4475	7.1550	1.4091	7.6447	1.6580	7.1552	1.4112
50	6.2813	1.1960	6.6966	1.1677	6.6896	1.1395	6.7032	1.1927	6.6962	1.1649	7.1461	1.3708	6.6964	1.1663
51	5.8936	9.8897(-5)	6.2758	9.6850(-5)	6.2704	9.4807(-5)	6.2810	9.8675(-5)	6.2756	9.6659(-5)	6.6893	1.1372	6.2757	9.6755(-5)
52	5.5371	8.2106	5.8894	8.0619	5.8851	7.9135	5.8935	8.1958	5.8892	8.0490	6.2702	9.4645(-5)	5.8893	8.0555
53	5.2087	6.8427	5.5338	6.7345	5.5304	6.6264	5.5370	6.8328	5.5337	6.7258	5.8849	7.9025	5.5337	6.7301

polation polynomial, the central point being that closest to z_0 or z_m. For cases where z_0 or z_m is about zero, this may involve calculations of $V(z)$ for negative z, and these are included in the Table.

APPENDIX C: RESULTS OF THE 100s LATTICE SUMS

In Table VI we present the results of the lattice sums on the 100s face at each of the four positions in Fig. 2(c) as functions of z; the coordinates, relative to the axes in Fig. 2(c), of each position, are in Table I.

The sums are calculated by the same method as described in Appendix B, except that the criterion for the choice of l is that *six* significant figures may be obtained for S_6, as it was originally intended to present this Table to six figures; this results in more than ten significant figures for S_{12}. As before, the complete range of z is separated into five smaller ranges, this time by $z/a = 0.5$, 1, 1.5, and 2. The values of l_0 and l_1 appropriate here are $l_0/a = 13$, 21, 31, 36, and 46, and $l_1/a = 18$, 30, 50, 50, and 60, respectively. All results are rounded to five significant figures, and all figures quoted, both in S_6 and S_{12}, are correct. For reasons similar to those in Appendix B, some calculations of $V(z)$ for negative z are done, and these are included.

TABLE VI. Results of the sums for the (100) simple cubic lattice face.

$20z/a$	$S_6(100s1,z)$	$S_{12}(100s1,z)$	$S_6(100s2,z)$	$S_{12}(100s2,z)$	$S_6(100s3,z)$	$S_{12}(100s3,z)$	$S_6(100s4,z)$	$S_{12}(100s4,z)$
-4					2.9211(1)	1.6319(2)		
-3					3.1311	1.9782		
-2					3.2985	2.2815		
-1					3.3997	2.4902		
0	∞	∞	5.2350(2)	2.6218(5)	3.4178	2.5639	1.3213(2)	8.1936(3)
1	6.4000(7)	4.0960(15)	4.9357	2.3281	3.3459	2.4873	1.2807	7.7186
2	1.0000(6)	1.0000(12)	4.1701	1.6523	3.1885	2.2752	1.1736	6.4755
3	8.7797(4)	7.7073(9)	3.2152	9.7134(4)	2.9600	1.9673	1.0217	4.8857
4	1.5630	2.4414(8)	2.3175	4.9580	2.6814	1.6143	8.5101(1)	3.3633
5	4.1007(3)	1.6777(7)	1.6001	2.3033	2.3760	1.2636	6.8410	2.1483
6	1.3761	1.8817(6)	1.0807	1.0140	2.0651	9.4896(1)	5.3544	1.2954
7	5.4794(2)	2.9593(5)	7.2569(1)	4.3624(3)	1.7659	6.8794	4.1144	7.4928(2)
8	2.4773	5.9606(4)	4.9004	1.8750	1.4903	4.8437	3.1266	4.2159
9	1.2367	1.4504	3.3529	8.1696(2)	1.2449	3.3315	2.3641	2.3343
10	6.6908(1)	4.0971(3)	2.3347	3.6427	1.0322	2.2504	1.7872	1.2837
11	3.8726	1.3060	1.6581	1.6715	8.5154(0)	1.5000	1.3558	7.0616(1)
12	2.3749	4.6006(2)	1.2019	7.9166(1)	7.0051	9.9076(0)	1.0349	3.9064
13	1.5316	1.7632	8.8880(0)	3.8755	5.7570	6.5075	7.9646(0)	2.1816
14	1.0322	7.2634(1)	6.6993	1.9613	4.7339	4.2632	6.1871	1.2334
15	7.2313(0)	3.1861	5.1401	1.0255	3.8998	2.7926	4.8550	7.0726(0)
16	5.2402	1.4772	4.0087	5.5330(0)	3.2219	1.8327	3.8494	4.1188
17	3.9112	7.1952(0)	3.1734	3.0765	2.6716	1.2070	3.0840	2.4378
18	2.9950	3.6642	2.5464	1.7598	2.2248	7.9882(−1)	2.4961	1.4669
19	2.3450	1.9430	2.0687	1.0338	1.8615	5.3176	2.0401	8.9758(| 1)
20	1.8715	1.0691	1.6994	6.2261(−1)	1.5654	3.5634	1.6832	5.5837
21	1.5186	6.0852(−1)	1.4103	3.8373	1.3232	2.4052	1.4011	3.5306
22	1.2500	3.5736	1.1813	2.4164	1.1245	1.6360	1.1760	2.2681
23	1.0418	2.1599	9.9789(−1)	1.5521	9.6064(−1)	1.1217	9.9484(−1)	1.4797
24	8.7780(−1)	1.3405	8.4950	1.0156	8.2500	7.7546(−2)	8.4774	9.7975(−2)
25	7.4669	8.5247(−2)	7.2835	6.7591(−2)	7.1217	5.4056	7.2733	6.5805
26	6.4054	5.5439	6.2858	4.5705	6.1787	3.7998	6.2799	4.4805
27	5.5361	3.6803	5.4577	3.1364	5.3866	2.6935	5.4543	3.0906
28	4.8170	2.4896	4.7654	2.1819	4.7180	1.9252	4.7634	2.1585
29	4.2168	1.7134	4.1826	1.5375	4.1510	1.3875	4.1815	1.5254
30	3.7116	1.1980	3.6890	1.0963	3.6678	1.0080	3.6883	1.0901
31	3.2834	8.4987(−3)	3.2683	7.9057(−3)	3.2541	7.3819(−3)	3.2679	7.8728(−3)
32	2.9180	6.1097	2.9079	5.7607	2.8983	5.4480	2.9077	5.7434
33	2.6043	4.4462	2.5975	4.2392	2.5910	4.0513	2.5974	4.2300
34	2.3334	3.2723	2.3289	3.1486	2.3245	3.0350	2.3288	3.1437
35	2.0984	2.4335	2.0953	2.3590	2.0923	2.2900	2.0953	2.3564
36	1.8935	1.8272	1.8914	1.7821	1.8894	1.7399	1.8914	1.7807
37	1.7140	1.3843	1.7126	1.3568	1.7112	1.3308	1.7126	1.3560
38	1.5562	1.0575	1.5553	1.0406	1.5543	1.0246	1.5553	1.0402
39	1.4169	8.1412(−4)	1.4163	8.0373(−4)	1.4157	7.9380(−4)	1.4163	8.0350(−4)
40	1.2936	6.3135	1.2931	6.2491	1.2927	6.1872	1.2931	6.2478
41	1.1839	4.9297	1.1836	4.8896	1.1833	4.8509	1.1836	4.8889
42	1.0861	3.8740	1.0859	3.8489	1.0857	3.8246	1.0859	3.8485
43	9.9869(−2)	3.0629	9.9855(−2)	3.0472	9.9841(−2)	3.0319	9.9855(−2)	3.0470
44	9.2026	2.4356	9.2016	2.4257	9.2007	2.4160	9.2016	2.4256
45	8.4972	1.9474	8.4965	1.9411	8.4959	1.9349	8.4965	1.9410
46	7.8612	1.5651	7.8607	1.5611	7.8603	1.5572	7.8607	1.5610
47	7.2863	1.2640	7.2859	1.2615	7.2856	1.2590	7.2859	1.2615
48	6.7654	1.0257	6.7652	1.0241	6.7649	1.0225	6.7652	1.0241
49	6.2924	8.3609(−5)	6.2922	8.3505(−5)	6.2921	8.3402(−5)	6.2922	8.3504(−5)
50	5.8619	6.8444	5.8618	6.8377	5.8617	6.8311	5.8618	6.8377