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SURFACE DISTORTION IN FACE-CENTERED CUBIC SOLIDS

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Until now, experimental values have not been obtained for the displacement of the surface layers from the bulk of semi-infinite crystals; such information will probably soon be available from Low Energy Electron Diffraction (LEED) studies. It is desirable to have some theoretical estimation of the order of magnitude of the displacements.

Gazis and Wallis[1] have shown that a one dimensional lattice with

[1] D.G. Gazis and R. F. Wallis, Surf. Sci. 3, 19 (1964).

nearest and next-nearest neighbor interactions may exhibit a distortion of the lattice spacing at a free surface; the predicted distortion decreases exponentially with distance from the surface.

Shuttleworth[2] has calculated the displacement of the first layer of

[2] R. Shuttleworth, Proc. Roy. Soc. (London) A62, 167 (1949).

the (100) surface of argon and Alder, Vaisnys, and Jura[3] have calculated

[3] B.J. Alder, J.R. Vaisnys, and G. Jura, J. Phys. Chem. Solids, 11, 182 (1949).

the displacements of the first five layers of the (100) surface of argon. Alder et al. found that the distortion decreased proportionally to the inverse cube of the distance from the surface.

The values of the coefficients in the Morse potential

$$\phi(r) = D[e^{-2\alpha(r-r_o)} - 2e^{-\alpha(r-r_o)}]$$

were tabulated by Girifalco and Weizer[4] for six fcc metals, Ca, Ag, Al,

[4] L. A. Girifalco and V. G. Weizer, Phys. Rev. 114, 687 (1959).

Pb, Cu, and Ni (Table 1). We have calculated the displacements, δ_1 (Fig. 1) of the first two surface layers of these metals for the (100), (110), and (111) surfaces. For comparison purposes we have also calculated the same displacements for argon using a Lennard-Jones 6-12 potential.[5]

[5] T. Kihara, J. Phys. Soc. Japan, 3, 265 (1948).

The surface energy, without allowing for distortion E_o, was calculated for each case considered by direct summation over a lattice of 2000 atoms. The surface energy was then minimized with respect to the displacements, δ_i, by direct summation of the energy over a lattice of 360 atoms on a CDC 6600 computer.

The surface energies without relaxation, E_o, the displacements, δ_i, and the changes in surface energy due to relaxation, ΔE, are tabulated in Tables 2, 3, and 4 for the (100), (110), and (111) surfaces respectively. The displacements, δ_i, are given in units of percentage of the normal bulk planar spacing. The values of Alder et al. are included in Table 2.

The results of Alder et al.[3] are based on direct summation of the energy over a lattice of roughly forty thousand atoms and integration over the remainder of the lattice; our results are based on only 360 atoms. Comparison of Alder's results with ours shows that this small lattice yields good values of δ_1, δ_2 and ΔE. Alder's work shows that consideration of the relaxation of only two surface layers gives good values of the surface energy.

For all the materials considered, it was found that the (111) surface was the lowest energy surface and the (110) the highest; distortion was largest for the (100) surface and smallest for the (111) surface. Relaxations were found to alter the surface energy by at most 6% and only slightly affected the ratios of the surface energies of the various faces.

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TABLE 1

Parameters of Morse Potential

$$\phi(r) = D[e^{-2\alpha(r-r_o)} - 2e^{-\alpha(r-r_o)}]$$

Metal	$\alpha(\mathring{A}^{-1})$	$r_o(\mathring{A})$	D(ev)
Pb	1.1836	3.733	.2348
Ag	1.3690	3.115	.3323
Ni	1.4199	2.780	.4205
Cu	1.3588	2.866	.3429
Al	1.1646	3.253	.2703
Ca	.80535	4.569	.1623

TABLE 2

The (100) Surface: Relaxations, δ_i, are given as a percentage of the bulk (100) planar spacing; E is the unrelaxed (100) surface energy; ΔE is the change in surface energy due to relaxation.

Solid	$\delta_1(\%)$	$\delta_2(\%)$	E_o(ev)	ΔE(ev)
Ca	12.504	3.587	.99925	-.06556
Ag	6.456	1.259	1.30302	-.03755
Al	10.972	2.963	1.49150	-.08410
Pb	5.542	.978	.85209	-.02011
Cu	9.669	2.433	1.72345	-.08319
Ni	9.121	2.232	2.02644	-.09119
Ar	2.604	.623	.039021	-.000355
Ar*	2.577	.589	.03951	-.000349

* Obtained by Alder et al.[3]

TABLE 3

The (110) Surface: Relaxations, δ_i, are given as a percentage of the bulk (110) planar spacing; E is the unrelaxed (110) surface energy; ΔE is the change in surface energy due to relaxation.

Solid	δ_1(%)	δ_2(%)	E_o(ev)	ΔE(ev)
Ca	9.621	2.628	1.45532	-.08664
Ag	4.783	.768	1.93619	-.04494
Al	8.362	2.099	2.18216	-.10898
Pb	4.075	.559	1.27073	-.02347
Cu	7.314	1.671	2.53181	-.10587
Ni	6.872	1.507	2.98250	-.11498
Ar	1.809	.366	.05779	-.000394

TABLE 4

The (111) Surface: Relaxations, δ_i, are given as a percentage of the bulk (111) planar spacing; E is the unrelaxed (111) surface energy; ΔE is the change in surface energy due to relaxation.

Solid	δ_1(%)	δ_2(%)	E_o(ev)	ΔE(ev)
Ca	4.297	.899	.87518	-.02558
Ag	1.910	.225	1.11727	-.01087
Al	3.667	.709	1.30167	-.03111
Pb	1.580	.159	.72635	-.00539
Cu	3.142	.544	1.49844	-.02913
Ni	2.927	.490	1.75856	-.03114
Ar	.820	.190	.032520	-.000113

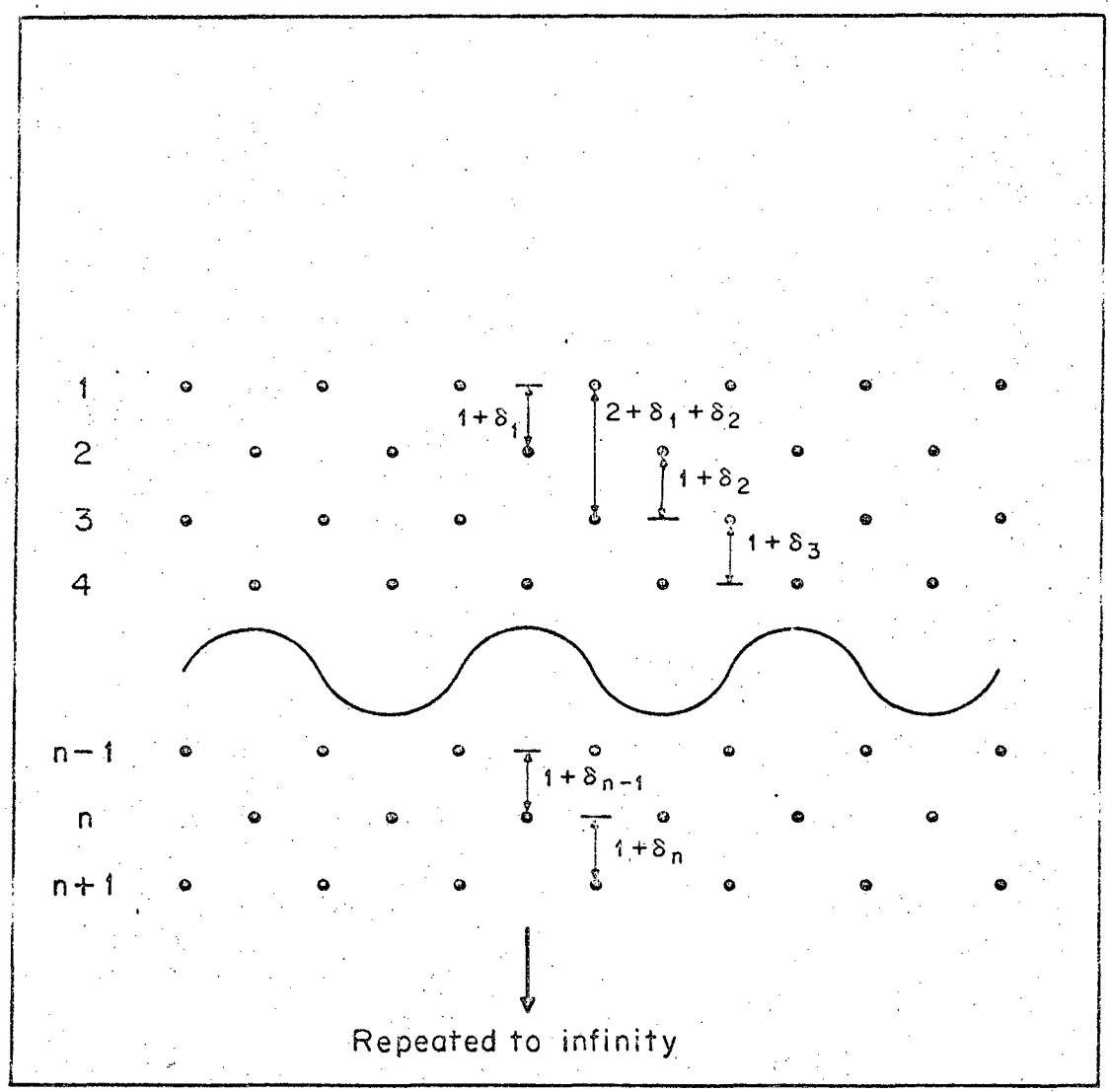

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Fig. 1 Schematic diagram of a semi-infinite crystal with displacements indicated

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