Table 1. *Ratio of the nearest-neighbour distance, r_1*, for minimum lattice energy to the distance of the minimum in the potential function, r_0. For ratios of lattice parameter to r_0, the values given must be multiplied by $\sqrt{2}$ for face-centred cubic and $2/\sqrt{3}$ for body-centred cubic crystals*

Face-centred cubic

Morse a =	3	3·5	4	4·5	5	6
r_1^*/r_0	0·6346	0·8266	0·9014	0·9395	0·9612	0·9825
Mie m =	4·5	5	6	7	8	9
n = 6	0·8140	0·8519				
7	0·8564	0·8873	0·9243			
8	0·8844	0·9104	0·9411	0·9583		
10	0·9182	0·9379	0·9607	0·9731	0·9806	0·9855
12	0·9375	0·9532	0·9712	0·9809	0·9866	0·9903
14	0·9497	0·9628	0·9776	0·9855	0·9901	0·9930

Body-centred cubic

Morse a =	3	3·5	4	4·5	5	6
r_1^*/r_0	0·6167	0·8035	0·8767	0·9147	0·9367	0·9601
Mie m =	4·5	5	6	7	8	9
n = 6	0·7932	0·8303				
7	0·8351	0·8655	0·9021			
8	0·8629	0·8886	0·9193	0·9368		
10	0·8974	0·9169	0·9399	0·9529	0·9611	0·9666
12	0·9178	0·9335	0·9519	0·9621	0·9686	0·9730
14	0·9312	0·9444	0·9597	0·9682	0·9736	0·9772

Table 3. *Temperatures and pressure necessary to change lattice parameters by particular amounts*[11,12]

Material	Temperature (°K) at which the lattice parameter exceeds 0°K value by		Pressure (10^3 kg/cm²) which changes the lattice parameter at room temperature by		
	1 per cent	2 per cent	−0·5 per cent	−1 per cent	−2 per cent
Na	180	350	1·0	2·0	4·2
Al	450	800	11·5	25	57
Cu	650	1250	23·5	53	~200
W	1950	3250	70	—	—

considered in terms of temperature or pressure, Table 3 gives the relevant experimental data for a few metals.

3. RESULTS

Table 4 shows the calculated lattice energy for various potentials together with the variations expected for 1 per cent and 2 per cent change in parameter.

Since E_G has been minimized at r_1*, the changes in the total lattice energy are all small but much greater changes occur in the energies associated with the interactions of particular atoms or groups of atoms. Thus, Fig. 2 shows, for a Morse $a = 4$

Table 2. *Constants in the Morse potential as deduced by* Girifalco *and* Weizer.[3] *The expressions in brackets use the symbols from* (3)

Metal	Face-centred cubic crystals											
	Cu	Al	Ca	Sr								
$E_0(=D)$, in eV	0·3429	0·2703	0·1623	0·1513								
$a(=\ln\beta)$	3·894	3·788	3·680	3·680								
$r_1^*/r_0\ (=\sqrt{2}\alpha a_0/\ln\beta)$	0·8898	0·8762	0·8602	0·8602								
Metal	Body-centred cubic crystals											
	Fe	Ba	K	Na	Cs	Rb	Pb	Ag	Ni			
$E_0(=D)$, in eV	0·4174	0·1416	0·05424	0·06334	0·04485	0·04644	0·2348	0·3323	0·4205			
$a\ (=\ln\beta)$	3·951	3·530	3·170	3·148	3·142	3·098	4·419	4·265	3·947			
$r_1^*/r_0\ (=\sqrt{3}\alpha a_0/\ln\beta)$	0·8716	0·8096	0·7065	0·6972	0·6947	0·6743	0·9348	0·9244	0·8958			
Metal	Mo	Cr	W									
$E_0(=D)$, in eV	0·8032	0·4414	0·9906									
$a\ (=\ln\beta)$	4·488	4·330	4·279									
$r_1^*/r_0\ (=\sqrt{3}\alpha a_0/\ln\beta)$	0·9140	0·9041	0·9006									