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## Density-dependent potentials for simulations

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**Abstract.** We have obtained a simple analytic pair potential and volume potential for simulations of simple metals in which the density dependence of the parameters is given explicitly. The potentials are based on a first-principles non-local pseudopotential theory with a correction term in the volume potential to allow for the effects of the density dependence of terms in the total energy beyond second order in perturbation theory. This correction term gives the pressure required to obtain the measured equilibrium lattice constant. In this paper we present a potential for Li and show that it gives the FCC structure at low temperatures, and gives good agreement with measured phonon dispersion curves and elastic constants.

### 1. Introduction

This paper derives a simple analytic pair potential,  $\varphi$ , and a volume potential,  $\bar{U}_0$ , for use in simulations of simple metals. These potentials are derived from a non-local pseudopotential theory presented in the preceding paper (Walker and Taylor 1990), hereafter referred to as paper I, based on the theory of Dagens *et al* (DRT) (Rasolt and Taylor 1975, Dagens *et al* 1975). The motivation for creating such potentials is to provide a potential based on first-principles theory that is simple enough to be used in constant-pressure simulations where the mean density, and hence the effective interaction, is allowed to vary, and also in simulations of defective systems where the density may vary locally. An important reason for using the DRT potentials is that they have given excellent results for defects and disorder in metals such as Al (Jacucci *et al* 1981). Such first-principles potentials have the correct functional form for the long-range Friedel oscillations, which appear to be critical in obtaining the correct atomic structure at the grain boundaries between bicrystals (V Vitek, private communication). The advantage that these potentials have over the embedded atom method (EAM) is that such features as the Friedel oscillations are automatically present in these potentials; in the EAM they would have to be specially inserted.

This point is emphasized when the variable cell molecular dynamics, devised by Parrinello and Rahman (1980), is applied to simulate metals under a constant external pressure. Here the cell's shape and size and hence the mean density of the system are determined by the balance between the externally applied stress and the internal stress generated by the ions and conduction electrons. The latter arises both from the variation with density of the volume and structural terms in the energy and from the motions of

the ions (Walker *et al* 1986). Munro and Mountain (1983) and Walker *et al* (1986) simulated the phase diagram of Li with the variable cell technique, employing potentials based on pseudopotential theory. The first two authors, however, did not include the pressure term arising from the volume term.

In a recent application of variable cell molecular dynamics, Cagin and Ray (1988) found that the density dependence of the metallic potentials is important in the calculation of elastic constants. Furthermore, Rosenfeld and Stott (1987) were able to show that the discrepancy between elastic constants from the long-wavelength limit of the acoustic phonons and from homogeneous deformation 'compressibility problem' arises from the sensitivity of the pair potentials to inhomogeneities in the electron density arising from the phonons.

The density dependence of the interactions of metals is also important for their disorder and defect properties, e.g. the vacancy formation energy (Jacucci and Taylor 1979, Jacucci *et al* 1981) and grain boundary structures (Sutton 1984). The interatomic potentials are sensitive to the local depletion of charge near the defect as there are changes in the density of electrons screening the ions. Finnis and Sachdev (1976) tried to predict corrections to the vacancy formation energy by letting the density refer to the local atomic environment but found the corrections to be too small to explain discrepancies between their theory, based on a local Ashcroft pseudopotential, and experiment.

We have adapted the approach of Pettifor and Ward (1984) to fit the effective pair potential,  $\varphi_{\text{DRT}}$ , of DRT to a sum of four exponentially decaying oscillatory terms. This functional form was found to be the simplest way of reproducing  $\varphi$  sufficiently well that, in common with DRT's potential, the FCC structure is predicted to be lower in energy for Li than the BCC at low temperatures. (Note that we have not performed calculations for the 9R structure, the observed (Overhauser *et al* 1984) low-temperature phase of Li.) This is a stringent test of our fitting procedure, given that the difference between the energies for different structures is of the order of 0.003 eV/ion and so a few per cent of the total energy. We have fitted each parameter in the potential to a quadratic in the density, a procedure that gives fits accurate to 0.1% over a range of densities from 0.9 to 1.1 times the standard density in the calculations presented here.

A quadratic fit for the density dependence of  $\bar{U}_0$  has been found from the formalism presented in paper I but with the approximation that the energy-wavenumber characteristic  $F(q)$  is represented by a Padé approximant, the same approximation used to obtain a Pettifor-Ward form for  $\varphi$ . The quadratic includes an extra term,  $U_{\text{HO}}$ , whose origin is discussed in paper I. This term contains the only adjustable parameter in our theory due to the complexity of the first-principles calculations required to ascertain its exact magnitude. The adjustable parameter is fixed such that  $U_{\text{HO}}$  gives the correct equilibrium volume.

In this paper we present results for Li, although similar potentials will be produced for the other simple metals in forthcoming publications. Section 2 describes how  $\varphi_{\text{DRT}}$  is fitted to a Pettifor-Ward-like potential  $\varphi$  and section 3 shows how an approximation to  $\bar{U}_0$  is found and gives tables of the coefficients for the quadratics used to fit the density dependence of  $U_0$  and the parameters in  $\varphi$ . Results are presented in section 4, and section 5 concludes the paper.

## 2. Effective pair potential

In paper I (equation (2.24)) it is shown that  $\varphi$  depends on  $F(q)$  as follows:

$$\varphi(r) = [Z^2 e^2 / (4\pi\epsilon_0 r)] \left( 1 - (2/\pi) \int_0^\infty F(q) [\sin(qr)/q] dq \right). \quad (2.1)$$

If a Padé approximant, i.e. the ratio of two polynomials,  $A(q^2)$  and  $B(q^2)$ , where  $B(q^2)$  is of order  $n$ , is used for  $F(q)$ , then

$$F(q) = 1 - q^2 \sum_{i=1}^n D_i / (q^2 - q_n^2) \quad (2.2)$$

where

$$D_i = A(q_n^2) / \left( \sum_{j \neq i} (q_j^2 - q_i^2) \right) = d_i \exp(i\delta) \quad (2.3)$$

and  $i$  and  $j$  run over all the roots of  $B(q^2)$ . Various values of  $n$  were tried, and the minimum value found to be 8 to give a pair potential that produces a lower energy for FCC than BCC for Li at zero temperature and at a standard density derived from a lattice constant of 3.478 Å for a BCC lattice (Beg and Nielsen 1976). There were three complex conjugate pairs of roots and two real roots at all the densities (i.e.  $0.9\rho_0$  to  $1.1\rho_0$  where  $\rho_0$  is the equilibrium density) for which  $F(q)$  was fitted. The amplitude  $A$  for the second real root was found to be less than 0.001% at all densities considered and is therefore ignored.

Thus from equation (2.1),

$$\varphi(r) = [Z^2 e^2 / (4\pi\epsilon_0 r)] \left( \sum_{i=1}^3 A_i \cos(k_i r + \alpha_i) \exp(-\kappa_i r) + A_4 \exp(-\kappa_4 r) \right) \quad (2.4)$$

where

$$q_i = k_i + i\kappa_i \quad q_4 = i\kappa_4 \quad (2.5)$$

$$A_i = 2d_i \quad A_4 = d_4. \quad (2.6)$$

Here  $i$  runs over the members of the complex conjugate pairs for which  $\kappa_i$  is positive.

Pettifor and Ward (1984) obtained the same form for  $\varphi$  for a local pseudopotential by approximating the Lindhard function  $f_0(q)$  by a ratio of two polynomials in  $q^2$  which reproduce  $f_0(q)$  for low and high values of  $q$ . Our approach is similar except that  $F(q)$  rather than  $f_0(q)$  is replaced by a Padé.

To fit  $F(q)$  to a Padé we used the expansion of  $F(q)$  for low  $q$  given in appendix 1 of paper I. Since appendix 1 of paper I also shows that, at large  $q$ ,

$$[1 - F(q)]/q^2 \approx 1/q^2 + O(1/q^6) \quad (2.7)$$

$A(q^2)$  has to be of order  $n - 1$ . The first three terms of  $A(q^2)$  are determined from the requirement that the Padé reproduces the low- $q$  expansion, equation (A1.18–20) of paper I to order  $q^6$ , and the two highest-order coefficients of  $A(q^2)$  are set equal to the two highest-order coefficients of  $B(q^2)$ . The remaining terms were obtained by a least-squares fit of (2.3) to  $F(q)$  calculated from the theory given in paper I at 51 points. In these calculations the approximation given in equation (A2.4) of paper I for the local field,  $\varphi_{LF}(0)$ , was used when calculating the susceptibility. As is clear from figure 3 and equation (A2.5) of paper I, which compares the approximate expression for the correlation factor  $F_C$  with the expression derived by Vosko *et al* (1980), this approximation will have a negligible effect on our results.

To find the density dependence of the parameters  $k_i$ ,  $\kappa_i$ ,  $A_i$  and  $\alpha_i$  for  $i = 1, 2, 3, 4$ , these parameters were calculated for 11 values of the density  $\rho$  in units of  $\rho_0$ , i.e.  $\rho = 0.90, 0.92, \dots, 1.1\rho_0$ , and fitted to a quadratic in  $\rho/\rho_0$  with coefficients  $Q_0, Q_1, Q_2$  defined from

$$Q(\rho/\rho_0) = Q_0 + (\rho/\rho_0 - 1)[Q_1 + Q_2(\rho/\rho_0 + 1)]. \quad (2.8)$$

A least-squares routine was used, which gave a deviation of typically 0.01% of the fitted values, the maximum deviation being 0.7% for a few values of  $Q_2$ .

### 3. Total theory

The density dependence of the total energy,  $U_{\text{tot}}$ , is required for the pressure generated by the conduction electrons. In this section we show how we have calculated and fitted  $\bar{U}_0$ , the volume energy corrected to take account of the core-conduction electron interaction  $U_{\text{HO}}$ , where

$$\bar{U}_{\text{tot}} = \bar{U}_0 + U_{\text{II}} \quad (3.1)$$

(equation (4.1) of paper I), and

$$U_{\text{II}} = (0.5/N) \sum'_{m,m'} \varphi(|\mathbf{R}_m - \mathbf{R}_{m'}|, \rho) \quad (3.2)$$

(equation (2.23) of paper I) where  $N$  is the number of ions,  $\mathbf{R}_m$  is the position of the  $m$ th ion and the prime on the summation excludes  $m = m'$ .

The volume term  $U_0$  was calculated using the same programs as those used to generate  $U_0$  in paper I and fitted to a quadratic using exactly the same procedure (and the same densities) as described in section 2 for the potential parameters. Our motivation for doing this is that the static bulk modulus gives reasonable agreement with experiment (see section 4 below). As in paper I it was necessary to add a term  $U_{\text{HO}}$  to correct for higher-order terms in the total energy neglected in the pseudopotential theory given in paper I.  $U_{\text{HO}}$  is fixed to give zero pressure at the observed low-temperature value for the lattice constant. Here, we have simply used the fact that  $U_{\text{HO}}$  varies linearly with  $(\rho/\rho_0 - 1)$  and so written

$$U_{\text{HO}} = U'_{\text{HO}}(\rho/\rho_0 - 1) \quad (3.3)$$

where the derivative of  $U_{\text{HO}}$  with respect to  $\rho/\rho_0$ ,  $U'_{\text{HO}}$ , was fitted to give zero pressure at the observed equilibrium density. To find  $U'_{\text{HO}}$ , we used the quadratic fit to  $U_0$  mentioned above to obtain the derivative of  $U_0$  with respect to  $\rho/\rho_0$ . From equation (3.2), the derivative of  $U_{\text{II}}$  with respect to  $\rho/\rho_0$  was found from

$$\begin{aligned} U'_{\text{II}} = 0.5 \sum_{n,i} N_n [\exp(-\kappa R_n)/R_n] & \{ [A'_i - A_i[\kappa'_i R_n - (\kappa R_n + 1)/(3\rho/\rho_0)]] \\ & \times \cos(k_i R_n + \alpha_i) - [k'_i R_n + \alpha'_i - R_n k_i/(3\rho/\rho_0)] A_i \\ & \times \sin(k_i R_n + \alpha_i) \} \end{aligned} \quad (3.4)$$

in terms of the derivatives of the potential parameters (denoted by primes) obtained

**Table 1.** Coefficients of quadratics used to fit potential parameters.

Parameter	$Q_0$	$Q_1$	$Q_2$
$\bar{U}_0$	-7.45268800	-0.70679758	0.34535241
$k_1$	-1.91491057	-0.62781834	0.11225943
$k_2$	-1.19004337	-0.00848164	-0.01759972
$k_3$	-2.13814916	-0.42632610	-0.10166748
$\kappa_1$	1.12697989	-1.60116365	0.78003658
$\kappa_2$	1.93711059	-1.18303429	0.73440769
$\kappa_3$	0.29580147	-2.13994944	0.94350295
$\kappa_4$	2.86915466	-5.67344985	3.12084931
$A_1$	0.47112040	-2.80902202	1.29827102
$A_2$	2.44213109	-5.96463205	3.24716854
$A_3$	0.00829335	-0.12953926	0.06241810
$A_4$	1.02188971	2.94806413	-1.39099579
$\alpha_1$	-2.86854363	0.77039869	-0.18691158
$\alpha_2$	1.39223261	2.03887398	-0.91097913
$\alpha_3$	-1.81228897	-0.10110970	0.36907974

from the quadratic fits, and the positions and coordination number of the  $n$ th nearest-neighbour shell  $R_n$  and  $N_n$  respectively. The quadratic fit for  $\bar{U}_0$ , i.e. the volume term corrected for the core–conduction electron interactions, was then found from

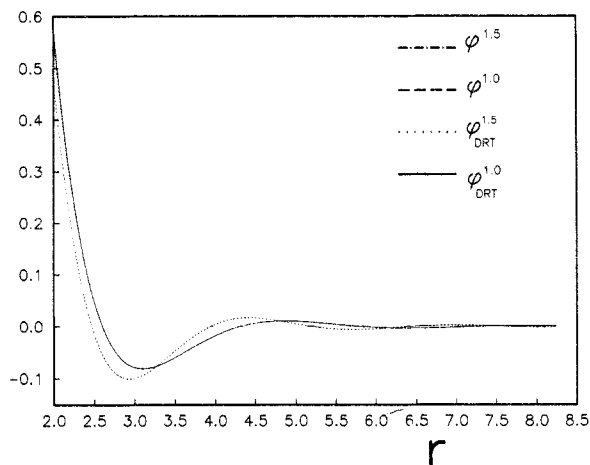
$$\bar{U}_0 = U_0 + U_{\text{HO}}. \quad (3.5)$$

#### 4. Results

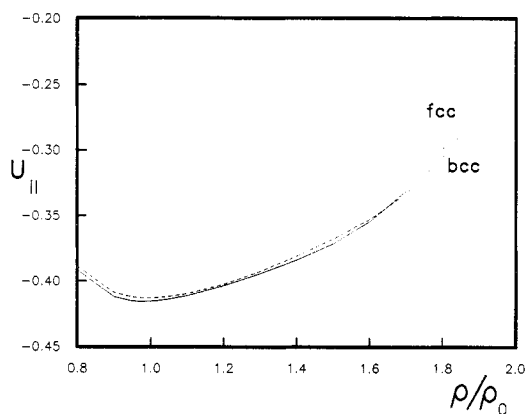
Table 1 gives the coefficients for the quadratic fits for  $\bar{U}_0$  and the potential parameters using the notation of equation (2.8). These coefficients can be supplied on request as a data file from either of the authors of this paper. They were calculated assuming a value of 4.382 Å in the FCC structure, equivalent to a BCC lattice constant of 3.478 Å, and the pseudopotential parameter values of DRT.

In figure 1 we have plotted  $\varphi(r)$  at  $\rho/\rho_0 = 1.0$  and 1.5, and compared our potential with the potential of DRT. The figure shows that our fitted potential is indistinguishable from DRT's potential in both cases. The closeness of this fit is essential to obtain the correct low-temperature structure.

We have calculated  $U_{\text{II}}$  as a function of the reduced density for the low-temperature FCC and BCC structures of Li with the fitted potential and presented our results in figure 2. We have not performed a calculation for the 9R structure, the low-temperature phase of Li (Overhauser 1984). Figure 2 shows that, while we have been able to produce a potential that gives FCC in preference to BCC at pressures up to about 15 GPa (from the pressure–density curve presented in figure 4), our potential favours the BCC structure at higher pressures. This last point disagrees with Olinger and Shaner (1983). On the other hand, the DRT potential gives FCC as the structure with the lower energy at all densities in the range shown in the figure. This discrepancy indicates that the fit to DRT's potential may not be sufficiently accurate to reproduce the correct structure at very high pressures.



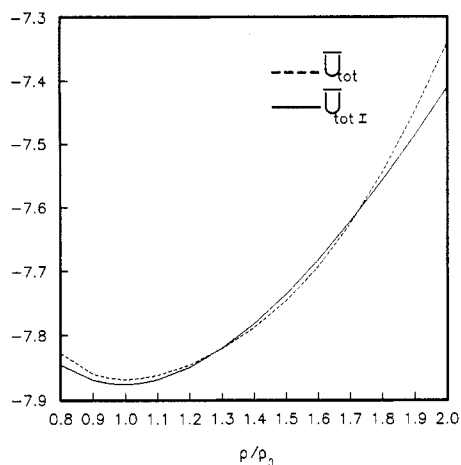
**Figure 1.** The pair potential  $\varphi$  and the pair potential  $\varphi_{\text{DRT}}$  of DRT (in eV) as a function of position  $r$  (in Å) for the densities  $\rho/\rho_0 = 1$  (broken curve and full curve respectively) and  $\rho/\rho_0 = 1.5$  (chain curve and dotted curve respectively).



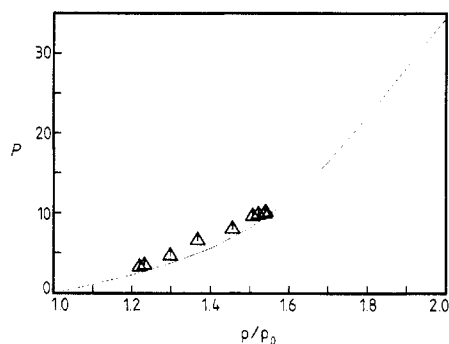
**Figure 2.** The structure-dependent contribution to the total energy,  $U_{\text{II}}$ , as a function of the density  $\rho$  in units of the equilibrium density  $\rho_0$  for the low-temperature FCC (full curve) and BCC (broken curve) structures. The units of  $U_{\text{II}}$  are eV.

However, it should be noted that the difference in energy is very small, e.g. 0.003 eV/ion at  $\rho/\rho_0 = 1$ . Hence, in consideration of this and the fact that we get good agreement between the two potentials over a wide range of pressure, we feel that we do have a very accurate fitting procedure.

Our concern in the foregoing was to provide a comparison between our potential and the DRT version. We recognize that the 9R structure is observed experimentally at low temperatures and that the FCC structure seems to exist in Li for only a narrow temperature range at moderate pressures (Smith *et al* 1990). We also note the comment of Smith *et al* (1990) that a search for the most stable structure should include the effects of vibrational entropy even at low temperatures, a question that is beyond the scope of this paper. Hence we have not at this stage concerned ourselves with identifying the predicted most stable structure for either our potential or that of DRT. Since 9R is similar to FCC, we have no reason to believe that either potential would give poor results.



**Figure 3.** The total energy corrected for the higher-order terms,  $\bar{U}_{\text{tot}}$ , for FCC as a function of  $\rho/\rho_0$ : results for fitted potential (broken curve), compared with the results from paper I,  $\bar{U}_{\text{tot},1}$  (full curve). The energies are given in eV.



**Figure 4.** The pressure  $P$  calculated for FCC as a function of  $\rho/\rho_0$  (full curve), compared with the room-temperature experimental measurements of Olinger and Shaner (1983) (triangles). The units of  $P$  are GPa.

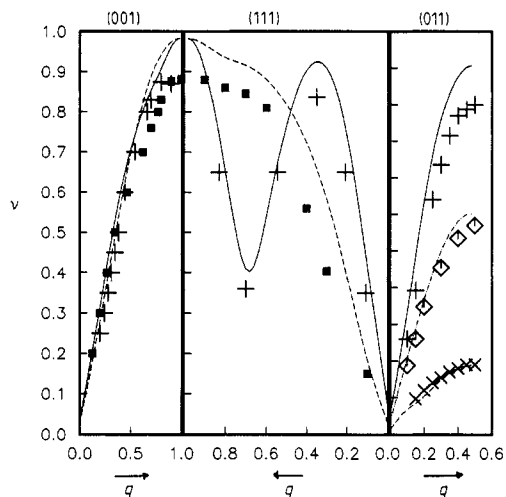
In figure 3 we have compared the total energy for an FCC structure as a function of  $\rho/\rho_0$  for the fitted potential ( $\bar{U}_{\text{tot}}$ ) and for the formalism presented in paper I ( $\bar{U}_{\text{tot},1}$ ). The difference between the two energies is largely due to the structural contribution  $U_{\text{II}}$  as the volume term  $\bar{U}_0$  for the fitted potential was obtained by fitting to the energy derived from the formalism in paper I. This figure shows just how sensitive  $U_{\text{II}}$  is to small differences in the pair potential, but the agreement is still within 0.02 eV up to  $\rho/\rho_0 = 1.8$ .

Figure 4 shows how the pressure depends on the density assuming a low-temperature FCC structure and compares our predictions with the room-temperature results of Olinger and Shaner (1983). Whilst Olinger and Shaner (1983) observe an FCC–BCC phase transition at a pressure of 7.5 GPa, this does not affect the density. The fact that we get such good agreement with Olinger and Shaner’s results is largely a consequence of obtaining reasonable agreement with the experimental value for the predicted static bulk modulus at  $\rho/\rho_0 = 1$  (see table 2 and the discussion of the results in it below).

The dispersion curves for the fitted potential are shown in figure 5 where they are compared with experimental values. We note that the agreement is as good for the DRT potential, but that it is not perfect, and would argue that the discrepancy has the origin discussed in some detail in DRT. Briefly, the discrepancy may arise from the very non-linear response due to the fact that the p components of the conduction electrons see the full ionic potential; from the possibility that three- and four-body forces play a significant role in the lattice dynamics; and from anharmonic effects due to Li being a light ion. The importance of anharmonic effects in Li has been noted by Taole *et al* (1978), who found significant shifts downward even at a temperature of 110 K. Such effects would be picked up when using these potentials in a molecular dynamics simulation.

In table 2 we have shown how the elastic constants from the phonon dispersion relations and the dynamic bulk modulus compare for our potential, the DRT potential





**Figure 5.** The predicted phonon dispersion curves from the fitted potential for BCC Li. The frequencies are in units of  $10^{13}$  Hz and the wavevector in units of  $2\pi/a$ , where  $a$  is the lattice constant. The full curves correspond to the longitudinal modes and the broken curves to transverse modes (in the (011) direction the broken curve corresponds to the  $T_1$  mode and the chain curve to the  $T_2$  mode). The points indicate the experimental results of Smith *et al* (1968): (+) for the longitudinal branches and (■) for the transverse branches (in the (011) direction (×) corresponds to the  $T_1$  mode and (◇) to the  $T_2$  mode).

**Table 2.** Elastic constants, bulk moduli and vacancy formation energy ( $E_{vac}$ ), a comparison between results for the fitted potential, the formalism in paper I and experiment. Results are presented for BCC and FCC structures as indicated. The elastic constants are obtained from the  $q \rightarrow 0$  limit of the phonon dispersion relations. The dynamic bulk moduli,  $B_{dynamic}$ , are equal to  $(C_{11} + 2C_{12})/3$  and the static bulk moduli,  $B_{static}$ , are equal to  $\Omega d^2 \tilde{U}_{tot}/d\Omega^2$ . The calculated  $E_{vac}$  are for an unrelaxed system. Note that at zero temperature the formation enthalpy at constant pressure, the measured  $E_{vac}$ , is equal to the formation energy at constant volume (Jacucci and Taylor 1979).

	Fitted potential	Formalism in paper I	Experiment
$C_{11}$ (GPa) (BCC)	16.2	18.0	18.0 <sup>a</sup>
$C_{12}$ (GPa) (BCC)	12.1	12.2	14.0 <sup>a</sup>
$C_{44}$ (GPa) (BCC)	10.4	11.1	12.0 <sup>a</sup>
$B_{dynamic}$ (GPa) (BCC)	13.5	14.1	15.3 <sup>a</sup>
$B_{static}$ (GPa) (FCC)	10.9	10.5	13.1 <sup>b</sup>
$B_{static}$ (GPa) (BCC)	10.5		11.6 <sup>b</sup>
$E_{vac}$ (eV) (BCC)	0.52	0.49	

<sup>a</sup> Beg and Nielsen (1976) at a temperature of 110 K.

<sup>b</sup> Olinger and Shaner (1983) at a temperature of 296 K.

and experiment. It should be noted that there is some uncertainty in the experimental value for the dynamic bulk modulus; the value quoted in the table comes from the elastic constants published by Beg and Nielsen (1976), who obtained their values from the low-energy phonons. These authors point out that their values are up to 20% higher than

the values obtained by a sound echo technique (Nash and Smith 1959). The discrepancy in the elastic constants from our potential and from the DRT potential is likely to be due to the damping out of the oscillations in the potential at long distances. This damping gives rise to errors in quantities like  $[e \cdot (q + G)/|q + G|]^2 F(|q + G|) - (e \cdot G/G)^2 F(G)$ , where  $G$  is a reciprocal lattice vector and  $e$  the polarization vector, which are evaluated when solving for the phonon frequencies. Anharmonic effects, discussed above, are likely to account for a large part of the disagreement with experiment.

Table 2 also shows the static bulk moduli  $B_{\text{static}}$  from the total energy obtained from using the fitted potential, the formalism in paper I and experiment. To obtain  $B_{\text{static}}$  from the formalism in paper I, the total energy was calculated at the same  $\rho/\rho_0$  values used for fitting the potential parameters (described in section 2 above) and these values for the total energy were fitted to a quadratic in  $\rho/\rho_0$ . We found that  $B_{\text{static}}$  from the formalism in paper I is very sensitive to the values of  $\rho/\rho_0$  used to fit the total energy, so that the result quoted in the table should only be regarded as giving an estimate. Given the difficulty of predicting an accurate value of  $B_{\text{static}}$ , the agreement with experiment is good. As  $B_{\text{static}}$  is not sensitive to  $U_{\text{HO}}$ , it is a useful test of the quality of the first-principles theory used. The origin of the difference between the dynamic and static bulk moduli has been discussed by Rosenfeld and Stott (1987). It is interesting to note that there is a quantitative difference here.

Finally, the unrelaxed vacancy formation energy reported in table 2 is a measure of the strength of the potential and should be roughly 10% greater than the experimental value. There is excellent agreement between the two potentials in this case, which is likely to be useful when we simulate defective metals using the fitted potential.

## 5. Conclusions

We have developed a very accurate fit to the first-principles potential of DRT and the volume energy of paper I, which contains the density dependence explicitly and is easy to use in a Monte Carlo or molecular dynamics simulation. Our potential predicts the FCC structure for Li up to pressures of 15 GPa. Our fit to the total energy produces bulk moduli, a pressure–density curve and phonon dispersion relations in good agreement with experiment. As our approach to obtaining an analytic fit to the pair potential requires only a means of calculating the energy–wavenumber characteristic, it could be used on any formalism where this quantity is derived.

Whilst results here are presented only for Li, work is in progress to generate potentials for other simple metals, which will be presented in future publications along with tests of the potential in molecular dynamics simulations.

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