LETTER TO THE EDITOR

Ab initio calculation of the elastic constants of magnesium

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Abstract. We have used a local, first principles pseudopotential to calculate the elastic constants of magnesium. Our results are in good agreement with experiment. The pseudopotential is obtained from the electronic density induced around a nucleus in an electron gas calculated from density functional theory.

The starting point in our approach [1–8] is the calculation of the displaced electron densities around a nucleus in an electron gas with an equilibrium density corresponding to magnesium. This was done using the density functional formalism [9, 10], and the model of the nucleus embedded into a jellium vacancy [1]. Taking into account that in the pseudopotential formulation the pseudodensity must not contain wiggles near the ion, these wiggles in the calculated density had to be removed [1, 8, 9].

We have used this approach successfully in previous work [3–8], to calculate from first principles the lattice specific heat and elastic constants of lithium, aluminium and its dependence on pressure and the phonon limited resistivity of aluminium, sodium and potassium.

We have used atomic units (i.e., magnitude of the electron charge = electron mass = $\hbar = 1$). The energy is given in double Rydbergs.

From pseudopotential theory and linear response theory [11], the interionic potential is given by

$$\Phi(r) = \frac{Z^2}{r}\left(1 + \frac{2}{\pi Z^2}\int \frac{\mathrm{d}q\,\sin(qr)\varepsilon(q)[\delta n(q)]^2}{q[1-\varepsilon(q)]}\right) \tag{1}$$

where r is the separation between the two ions, Z is the charge of the metal ion, $\varepsilon(q)$ is the dielectric response function of the electron gas and $\delta n(q)$ is the Fourier transform of the induced charge pseudodensity.

For the model of the nucleus embedded in a jellium vacancy, the induced electronic density is calculated by taking the difference [1]

$$\delta n(r) = n(r) - n_v(r) - 2\sum_b |\psi_b(r)^2| \tag{2}$$

where $n(r)$ is calculated with the total charge density corresponding to a nucleus located at the centre of a vacancy in jellium, and $n_v(r)$ is the electron density around a jellium vacancy alone. The bound states are given by ψ_b. Charge neutrality of the metal is a necessary condition.

The unscreened pseudopotential form factor, $\vartheta(q)$, is related to $\delta n(q)$ by

$$\vartheta(q) = \frac{4\pi \, \delta n(q) \varepsilon(q)}{q^2 [1 - \varepsilon(q)]}. \tag{3}$$

Equation (3) is used to obtain an effective local pseudopotential, which in linear response will give the exact induced displaced electronic density outside the region of smoothing. In this way some of the non-linear screening effects are included into the pair potential calculation from this pseudopotential.

The dielectric function we used satisfies by construction, the compressibility theorem which is important in connection with the interionic potential and it is given by [1, 12]

$$\varepsilon(q) = 1 + \left(\frac{4\pi}{q^2}\right) G(q) \tag{4}$$

where

$$G(q) = \frac{G_0(q)}{1 - (4\pi/k_{TF}^2) G_0(q)(1 - L)} \tag{5}$$

and $G_0(q)$ is the usual Lindhard polarizability, K_{TF} is the Fermi–Thomas screening constant, and L is the ratio

$$L = \left(\frac{\partial \mu}{\partial r_s}\right) \Big/ \left(\frac{\partial E_F}{\partial r_s}\right). \tag{6}$$

In equation (6) μ is the chemical potential, E_F is the Fermi energy and

$$\mu(r_s) = E_F(r_s) + \mu_{xc}(r_s) \tag{7}$$

where $\mu_{xc}(r_s)$ is the exchange–correlation contribution to the chemical potential.

Using the expression of Gunnarson and Lundquist [12], for exchange–correlation (which is the one we used in the calculation of the induced electronic density), the corresponding value of L is

$$L = 1 - \left(\frac{4}{9\pi}\right)^{1/3} r_s \left(1 + \frac{0.6213}{r_s + 11.4} r_s\right). \tag{8}$$

With the induced charge pseudodensity and the dielectric function already given, we used equation (1) to calculate the interionic potential.

From the interionic potential we calculated the phonons and associated force constants, using the harmonic approximation.

Magnesium has hexagonal close packed structure (HCP). For this structure, we had a good convergence with four neighbour shells. For this case the elastic constants, C_{11}, C_{44}, C_{12}, C_{33} and C_{13} are given by [13, 14]

$$C_{11} = \sqrt{3}(3\alpha A_1 - L)/(2c) \tag{9}$$

where

$$L = \frac{(2B_2 + G_2 + 3G_1)(3B_1 + B_2 + 8G_2) + 2G_2(3B_1 + B_2)}{3(B_1 + B_2 + G_1 + G_1)} \tag{10}$$

$$C_{33} = \frac{c}{\sqrt{3}a^2}[-3(B_3 + G_3) + 4\delta] \tag{11}$$

$$C_{44} = \frac{-2}{\sqrt{3}c}(3A_2 + B_3 + 4G_3) \tag{12}$$

$$C_{12} = \frac{-1}{\sqrt{3}c}[3(\alpha - 3A_1) - 3B_1 - B_2 - 12G_1 - 4G_2 + P] + C_{11} \tag{13}$$

where

$$P = \frac{(B_1 - B_2 - 2G_1 + 2G_2)^2}{B_1 + B_2 + G_1 + G_2} \tag{14}$$

$$C_{13} = \frac{2}{a}(2G_4 - B_4) - C_{44}. \tag{15}$$

In the case of an ideal HCP structure, $c/a = \sqrt{8/3}$.

The force constants and the derivatives of the interionic potential are related by [14]

$$\alpha = -[k_1(1) + C_B(1)] \quad A_1 = A_2 = C_B(1) \qquad A_3 = 0$$
$$B_1 = C_B(2) \qquad B_2 = (1/3)[k_1(2) + 3C_B(2)] \quad B_3 = 2B_2 - B_1$$
$$B_4 = \sqrt{2}(B_2 - B_1) \qquad G_1 = C_B(3) \qquad G_2 = (1/3)[2k_1(3) + 3C_B(3)]$$
$$G_3 = (1/2)(G_1 + G_2) \quad G_4 = (G_2 - G_1)/\sqrt{2} \qquad \delta = -[k_1(4) + C_B(4)]$$

where $k_1(S)$ and $C_B(S)$ are the two force constants of the axially symmetric model for the Sth shell of neighbours [15].

The force constants $k_1(S)$ and $C_B(S)$ are related to the derivatives of the interionic potential by [15]

$$k_1(S) = \left[\frac{d^2 V(r)}{dr^2} - \frac{1}{r} \frac{dV(r)}{dr} \right]_{(S)} \tag{16}$$

and

$$C_B(S) = \left[\frac{1}{r} \frac{dV(r)}{dr} \right]_{(S)}. \tag{17}$$

From the interionic potential we can find $k_1(S)$ and $C_B(S)$ and, from these, the corresponding elastic constants for HCP.
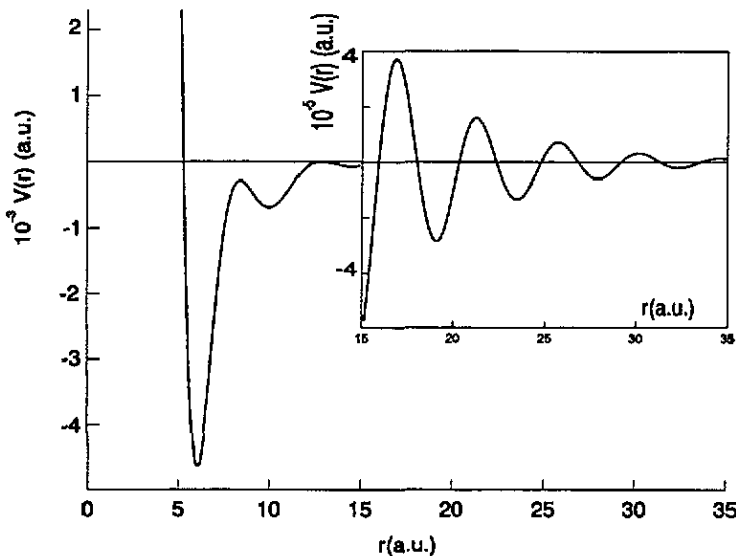

Figure 1. The resulting interionic potential.

In figure 1 we show the resulting interionic potential. From this interionic potential we calculated the derivatives to be used in order to obtain the elastic constants.

Table 1. Predicted elastic constants for magnesium. The experimental results are from [16]. This calculation is for 300 K (we are taking $r_s = 2.66 \, a_0$, where a_0 is the Bohr radius, $a_0 = 0.529$ Å). The units are 10^{11} dyn cm^{-2}.

	C_{44}	C_{11}	C_{12}	C_{33}	C_{13}
Experiment	1.827	8.260	3.160	9.746	1.880
Theory	1.642	5.943	2.560	6.164	2.140

Our calculated elastic constants are shown in table 1, where a comparison with experiment is made. We can see a good agreement, which gives us some confidence on the validity of our first principles pseudopotential for magnesium.

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