Lattice distortion around a vacancy in magnesium

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Using the D_{3h} point-group symmetry of an atom in magnesium and the defect-space matrix-partitioning technique, the perfect- and defect-crystral Green's functions are calculated in a two-neighbor defect-space model in an axially symmetric host lattice. The magnitude of the lattice distortions for the first two shells is found to be ~ 0.004 times the basal lattice constant, and the relaxation energy E_r of the vacancy is 0.0026 eV. Approximating the medium by an elastic continuum, but using values of the strength tensor corresponding to four different lattice models, the change in volume ΔV of the medium is found to vary from -0.03 to -0.11 times the atomic volume and the relaxation energy is found to vary from 0.0014 to 0.014 eV. In the above approximation, expressions for ΔV and E_r involving the bond-bending force constants are derived.

I. INTRODUCTION

In this paper we investigate the static relaxation of atoms surrounding a vacancy in magnesium applying the theory developed in the preceding paper[1] (hereafter referred to as I), retaining the same notation. We make the usual assumption[2] that if $V(r(n))$ is the pair potential between the atom labeled 0 at the origin and the nth atom at a distance $r(n)$, and if the former atom is removed to create a vacancy, then the effect of the vacancy on the nth atom can be described by $-V(r(n))$. We also assume that the potential $V(|\vec{r}(n)-\vec{r}(n')|)$ between any two atoms $(n\neq n'\neq 0)$ remains unchanged even in the presence of the vacancy. This implies that the forces (described by a $3p$-dimensional vector $\vec{f}$) responsible for the relaxation of the atoms are opposite to those acting on the (unrelaxed) atomic positions in the defect space, i.e.,

$$f_\alpha(n) = [(1/r)V'(r)]_n x_\alpha(n)\,, \tag{1.1}$$

where the prime denotes the derivative with respect to r and the subscript n indicates that the quantity is to be evaluated at $r=r(n)$.

The results of I are applicable to the present problem in the $\omega\to 0$ limit. In the presence of "applied" forces $\{\vec{f}(n)\}$, Eq. (2.1) of I becomes

$$(\underline{\phi}^s - \delta\underline{\phi}^s)\vec{u}^s = \vec{f}^s\,, \tag{1.2}$$

where $\vec{f}^s$ is the symmetry-reduced form of $\vec{f}$. This equation can be inverted to yield

$$\vec{u}^s = \underline{g}^{*s}\vec{f}^s\,, \tag{1.3}$$

where

$$\underline{g}^{*s} = (\underline{I}_s - \underline{g}\delta\underline{\phi})^{-1}\underline{g}\,. \tag{1.4}$$

Because of Eq. (1.1), $\vec{f}$ has the same symmetry as that of the lattice, and hence the only mode which contributes to the displacements is the completely symmetric mode associated with the irreducible representation (IR) $s=A_1'$. In this paper the index s stands for A_1' alone. The relaxation energy due to the vacancy is given by

$$E_r = \tfrac{1}{2}\vec{f}^s\cdot\vec{u}^s\,. \tag{1.5}$$

The results of the calculation of $\vec{u}^s$, E_r, and the volume change ΔV due to a single vacancy are presented in Sec. III for a two-neighbor axially symmetric (AS) model (M1) of the host crystal.

First approximations to $\vec{u}^s$ and E_r, denoted, respectively, by $\vec{w}^s$ and W_r, are obtained by using $\underline{g}^s$ (in place of $\underline{g}^{*s}$) in Eq. (1.3). In this case we have

$$\vec{w}^s = \underline{g}^s\vec{f}^s \tag{1.3a}$$

and

$$W_r = \tfrac{1}{2}\vec{f}^s\cdot\vec{w}^s\,. \tag{1.5a}$$

If one approximates the medium by an infinite isotropic elastic continuum (magnesium is the most isotropic of all the hcp crystals), then the elastic displacement field $\vec{w}^\infty(r)$ evaluated at the atomic positions [and denoted by $\vec{w}^\infty(n)$] is given in terms of the elastic strength Λ, the Lamé's constant λ_0, and the shear modulus μ_0 by the expression[3]

$$w_\alpha^\infty(n) = \frac{\Lambda}{4\pi(\lambda_0+2\mu_0)}\,\frac{x_\alpha(n)}{[r(n)]^3}\,. \tag{1.3b}$$

The relaxation energy in this approximation is

$$W_r^\infty = \tfrac{1}{2}\vec{f}^s\cdot\vec{w}^{\infty s}\,, \tag{1.5b}$$

where $\vec{w}^{\infty s}$ is the symmetry-reduced form of $\vec{w}^\infty$. In Sec. IV we present the calculation of $w^{\infty s}$, W_r^∞, and the approximate volume change ΔV^∞ due to the vacancy on the basis of M1 and three other models: (a) a three-neighbor AS model (M2); (b) a four-neighbor AS model proposed by Iyengar *et al.*[4]

(M3); and (c) a four-neighbor spline-fitted interatomic pair potential proposed by Doneghan and Heald[5] (M4). Explicit expressions involving the bond-bending force constants (BBC's) are also derived in Sec. IV for the computation of ΔV^{∞} and W_r^{∞}. The manner in which the BBC's and the bond-stretching force constants (BSC's) are obtained is described in Sec. II.

Since the size of the defect space D is larger in M2, M3, and M4 (the dimension of D is 57 in M2, and 63 in both M3 and M4) than in M1, the expressions for $\underline{g}^s$ and $\delta\underline{\phi}^s$ derived in I are no longer applicable to these models. Although atomistic computations of $\vec{u}^s$, ΔV and E_r are not done for M2, M3, and M4, the approximate calculations help in assessing the reliability of the atomistic calculations of M1 and in demonstrating the importance of the BBC's for point-defect calculations. These questions are discussed in Sec. V.

II. BBC'S AND BSC'S

The vectors $\vec{f}^s$, $\vec{u}^s$, $\vec{w}^s$, and $\vec{w}^{\infty s}$ are obtained as follows. Symmetry considerations show that the vector $\vec{v}$ $(=\vec{f}, \vec{u}, \vec{w}, \text{ or } \vec{w}^{\infty})$ has the form

$$\vec{v}(1)=\begin{bmatrix}0\\ v_1\\ v_2\end{bmatrix} \tag{2.1}$$

and

$$\vec{v}(7)=\begin{bmatrix}v_3\\ v_4\\ 0\end{bmatrix}.$$

Then $\vec{v}^s$ $(=\vec{f}^s$, etc.) is calculated from the equation

$$v^s(a)=\vec{\psi}^{sa1}\cdot\vec{v} \quad (a=1,2,3,4)$$

as

$$\vec{v}^s=6^{1/2}\begin{bmatrix}v_1\\ v_2\\ v_3\\ v_4\end{bmatrix} \tag{2.2}$$

and the relaxation energy, using Eq. (1.5), is

$$E_r=3(f_1u_1+f_2u_2+f_3u_3+f_4u_4). \tag{2.3}$$

Similar expressions are obtained for W_r and W_r^{∞} on replacing u by w and w^{∞}, respectively, in Eq. (2.3).

In M3 and M4, the forces and displacements for atoms on the third and the fourth shells have to be considered too, whereas for M2, these quantities have to be included for the third shell alone. Let the atom numbered 18 $[\vec{x}(18)=(0, 2a/\sqrt{3}, \frac{1}{2}c)]$ represent the third shell (which consists of six atoms) and the atom numbered 20 $[\vec{x}(20)=(0,0,c)]$ represent the fourth shell (which consists of two atoms). The general forms of the vectors $\vec{v}(18)$ and $\vec{v}(20)$ $(\vec{v}=\vec{f}, \vec{u}, \vec{w}, \text{ or } \vec{w}^{\infty})$ are

$$\vec{v}(18)=\begin{bmatrix}0\\ v_5\\ v_6\end{bmatrix} \text{ and } \vec{v}(20)=\begin{bmatrix}0\\ v_7\\ v_8\end{bmatrix}. \tag{2.4}$$

It can be shown easily that Eqs. (2.2) and (2.3), in this case, have to be generalized to the following:

$$\vec{v}^s=6^{1/2}\begin{bmatrix}v_1\\ v_2\\ v_3\\ v_4\\ v_5\\ v_6\\ 3^{-1/2}\cdot v_7\\ 3^{-1/2}\cdot v_8\end{bmatrix} \tag{2.5}$$

and

$$E_r=3\sum_{i=1}^{6}f_iu_i+(f_7u_7+f_8u_8). \tag{2.6}$$

(For M2, $f_7=f_8=0$.) Similar expressions are obtained for W_r and W_r^{∞}.

The shell radii r_i $(i=1,2,3,4)$ are

$$r_1=(1+\tfrac{3}{4}\gamma_0^2)^{1/2}a=0.9955a,$$
$$r_2=a,$$
$$r_3=(1+\tfrac{3}{16}\gamma_0^2)^{1/2}a=1.411a, \tag{2.7}$$

and

$$r_4=\gamma_0 a=1.622a \quad (\gamma_0=c/a).$$

The BBC's for these shells (i.e., $(1/r)V'(r)$ at $r=r_i$ for $i=1,2,3,4$) are denoted by β_B, α_B, γ_B, and δ_B. The BSC's (i.e., $V''(r)$ at $r=r_i$ for $i=1,2,3,4$) are denoted by β_s, α_s, γ_s, and δ_s.

These parameters for M2 are obtained by making use of the following expressions:

$$\gamma_c'=\frac{4a}{3\sqrt{2}\gamma_0}\left[\left(1+\frac{2}{3\gamma_0^2}\right)C_{44}+\left(1-\frac{2}{3\gamma_0^2}\right)C_{13}-\frac{4}{3\gamma_0^2}C_{33}\right], \tag{2.8a}$$

$$\beta_c'=(a/\sqrt{3}\gamma_0)(C_{44}+C_{13})-\gamma_c', \tag{2.8b}$$

$$\alpha_c=\tfrac{1}{3}[\tfrac{1}{2}\gamma_0 a\sqrt{3}(C_{11}+C_{12})-\beta_c'-4\gamma_c'], \tag{2.8c}$$

$$\beta_B+\gamma_B=\frac{a}{\gamma_0 2\sqrt{3}}(C_{44}-C_{13}), \tag{2.8d}$$

TABLE I. BBC's and BSC's for all models (dyn cm^{-1}).

	$M1$	$M2$	$M3$	$M4$
β_B	−284	327	543	−34
α_B	−144	332	700	−19
γ_B	0	−611	−1650	−318
δ_B	0	0	614	41
β_s	12562	10767	10789	11370
α_s	11204	10861	9992	12366
γ_s	0	599	2149	495
δ_s	0	0	303	−322

$$\gamma_B+\alpha_B=\tfrac{1}{3}\left[\tfrac{1}{4}\gamma_0 a\sqrt{3}\,(C_{44}-C_{13})-(\beta_B+\gamma_B)\right], \tag{2.8e}$$

$$\alpha_B+\beta_B=\tfrac{1}{8}\left[4\pi^2 M\nu_{\mathrm{LO}}(\vec{q}_{\max})-6\alpha_c-2\beta_c'\right]. \tag{2.9}$$

In these equations

$$\alpha_c=\alpha_s-\alpha_B, \tag{2.10a}$$

$$\beta_c'=\beta_s'-\beta_B'=(a/r_1)(\beta_s-\beta_B), \tag{2.10b}$$

$$\gamma_c'=\gamma_s'-\gamma_B'=(a/r_3)(\gamma_s-\gamma_B), \tag{2.10c}$$

and $\nu_{\mathrm{LO}}(\vec{q}_{\max})$ is the maximum frequency of the $[01\bar{1}0]$ longitudinal-optical phonon. Equations (2.1a)–(2.1e) are obtained by making use of a corrected version of Tables (3c) and (5c) of Ref. 4. The values used for the elastic constants at 298 °K, in units of 10^{12} dyn cm^{-2}, are[6]

$$\begin{aligned} &C_{11}=0.5943, \quad C_{33}=0.6164,\\ &C_{12}=0.256, \quad C_{44}=0.1642,\\ &C_{13}=0.214, \quad C_{66}=0.1691, \end{aligned} \tag{2.11}$$

and we take[7]

$$\nu_{\mathrm{LO}}(\vec{q}_{\max})=6.88 \text{ THz}.$$

The parameters for M1 are obtained from Eqs. (2.10b)–(2.10e) on setting $\gamma_B=\gamma_c'=0$, and those for M3 are taken from Iyengar *et al.*[7] For M4, these were calculated from the potential proposed by Doneghan and Heald.[5] In Table I we list the BBC's and the BSC's for all four models. The lattice dispersion, using the expression given in Table 5(c) of Ref. 4, was computed in the [0001] direction, for all the four models and agreement with the reported data[7] was reasonably good in each case.

In concluding this section, we note the following relations between the force components and the BBC's:

$$\begin{aligned} &f_1=-(a/\sqrt{3})\beta_B, \quad f_5=(2a/\sqrt{3})\gamma_B,\\ &f_2=-(c/2)\beta_B, \quad f_6=(c/2)\gamma_B,\\ &f_3=a\alpha_B, \quad f_7=0,\\ &f_4=0, \quad f_8=c\delta_B, \end{aligned} \tag{2.12}$$

III. LATTICE CALCULATIONS

The results of this section are based on M1 alone. The perfect-crystal Green's functions were calculated up to eight shells by using the expression[8]

$$g_{\alpha\beta}(l\kappa,l'\kappa')=\frac{-1}{NM}\sum_{\vec{q},j}\frac{W_\alpha(\kappa|\vec{q}j)W_\beta^*(\kappa'|\vec{q}j)}{\omega_j^2(\vec{q})}\times\exp\{i\vec{q}\cdot[\vec{x}(l\kappa)-\vec{x}(l'\kappa')]\}. \tag{3.1}$$

The computation of the eigenfrequencies $\omega_j(\vec{q})$ (j is the branch index) and the corresponding polarization vectors $\vec{W}$ was done by diagonalizing the dynamical matrix at $N=3960$ $\vec{q}$ points in the first Brillouin zone. The independent parameters[1] occurring in the Green's functions are tabulated in Table II. The following results are obtained for the various quantities of interest:

TABLE II. Perfect-crystal Green's-function parameters (units of 10^{-6} cm dyn^{-1}) for the representative atoms up to eight neighbors.

Shell number	S_1	S_2	S_3	S_4	S_5	S_6	A_4	A_5	A_6
0	25.270	25.270	21.945	0.0	0.0	0.0	0.0	0.0	0.0
1	8.1703	6.9396	8.1554	1.0662	0.8990	1.5571	0.0	0.0	0.0
2	8.7403	10.6550	5.6728	1.6581	0.0	0.0	−0.1291	0.0	0.0
3	5.7944	5.4261	4.5483	0.0	0.2256	0.0	0.0	0.0	0.0
4	4.5850	4.5850	5.3354	0.0	0.0	0.0	0.0	0.0	0.0
5	5.6340	5.1167	3.7783	1.0082	0.5718	0.4425	0.0	0.0	0.0
6	5.2703	7.3638	3.8555	0.0	0.0	0.0	0.0	0.0	0.0
7	4.0944	4.3662	4.4679	0.2354	0.6422	0.3708	0.1238	−0.1004	−0.1738
8	4.9237	6.0109	2.8130	0.9415	0.0	0.0	0.0101	0.0	0.0

$$g^s = \begin{bmatrix} 11.5630 & -1.4853 & -2.0777 & 0.4184 \\ -1.4853 & 19.0190 & 4.9379 & -1.7670 \\ -2.0777 & 4.9379 & 16.1730 & -0.1190 \\ 0.4184 & -1.7670 & -0.1190 & 11.8990 \end{bmatrix} (10^{-6}\ \text{cm dyn}^{-1}),$$

$$\delta\underline{\phi}^s = \begin{bmatrix} 4036 & -6068 & 0 & 0 \\ -6068 & 8240 & 0 & 0 \\ 0 & 0 & 11204 & 0 \\ 0 & 0 & 0 & -144 \end{bmatrix} (\text{dyn cm}^{-1}),$$

$$\underline{g}^s = \begin{bmatrix} 12.6640 & -3.8473 & -3.3811 & 0.6448 \\ -3.8473 & 23.8720 & 7.7647 & -2.2295 \\ -3.3811 & 7.7647 & 20.4160 & -0.3204 \\ 0.6448 & -2.2295 & -0.3204 & 11.9260 \end{bmatrix} (10^{-6}\ \text{cm dyn}^{-1}),$$

$$\vec{f}^s = \begin{bmatrix} 5.2634 \\ 7.3934 \\ -4.6224 \\ 0.0 \end{bmatrix} (10^{-6}\ \text{dyn}),$$

$$\vec{w}^s = \begin{bmatrix} 1.8531 \\ 3.4262 \\ -1.5323 \\ -0.3212 \end{bmatrix} \times 10^{-3}a, \qquad \vec{u}^s = \begin{bmatrix} 1.6772 \\ 3.7492 \\ -1.7059 \\ -0.3616 \end{bmatrix} \times 10^{-3}a.$$

$W^r = 0.00253$ eV, $E_r = 0.00267$ eV.

IV. SEMICONTINUUM CALCULATIONS

The parameters λ_0 and μ_0 are obtained by taking the Voigt average of the elastic-constant data for single crystals, Eq. (2.11):

$$\begin{aligned} \lambda_0 &= \tfrac{1}{15}(C_{11} + C_{33} + 5C_{12} + 8C_{13} - 4C_{44}) = 0.2364 \times 10^{12}\ \text{dyn cm}^{-2}, \\ \mu_0 &= \tfrac{1}{30}(7C_{11} - 5C_{12} + 2C_{33} + 12C_{44} - 4C_{13}) = 0.1742 \times 10^{12}\ \text{dyn cm}^{-2}. \end{aligned} \tag{4.1}$$

The strength Λ is defined as one-third of the trace of the strength tensor

$$\Lambda_{\alpha\beta} = \sum_n f_\alpha(n) x_\beta(n), \tag{4.2}$$

and is calculated in the four-neighbor model as

$$\underline{\Lambda} = a \begin{bmatrix} -\sqrt{3}f_1 + 3f_3 + 2\sqrt{3}f_5 & 0 & 0 \\ 0 & -\sqrt{3}f_1 + 3f_3 + 2\sqrt{3}f_5 & 0 \\ 0 & 0 & \gamma_0(-3f_3 + 3f_6 + 2f_8) \end{bmatrix}. \tag{4.3}$$

TABLE III. Displacement components w_{1-8}^{∞} for all models (units of $10^{-3}a$).

	$M1$	$M2$	$M3$	$M4$
w_1^{∞}	2.346	2.512	7.036	2.866
w_2^{∞}	3.295	3.528	9.883	4.026
w_3^{∞}	−4.008	−4.292	−12.020	−4.898
w_4^{∞}	0.0	0.0	0.0	0.0
w_5^{∞}	−1.648	−1.764	−4.942	−2.013
w_6^{∞}	−1.157	−1.239	−3.471	−1.414
w_7^{∞}	0.0	0.0	0.0	0.0
w_8^{∞}	−1.523	−1.631	−4.570	−1.862

The scalar strength to be used in the continuum calculations is thus

$$\Lambda = \tfrac{1}{3}a(-2\sqrt{3}f_1 - 3\gamma_0 f_2 + 6f_3 + 4\sqrt{3}f_5 + 3\gamma_0 f_6 + 2\gamma_0 f_8). \tag{4.4}$$

The expression for the volume change per atomic volume, i.e., $\Delta V^{\infty}/\Omega$ ($\Omega = \frac{1}{2}\sqrt{3}\gamma_0 a^3$ is the atomic volume), is found by using Eqs. (4.4) and (2.12) in Eshelby's formula,[3]

$$\Delta V^{\infty}/\Omega = \Lambda/\Omega(\lambda_0 + 2\mu_0) = \frac{2\sqrt{3}}{a\gamma_0}\,\frac{(\frac{1}{2}\gamma_0^2+1)\beta_B + 2\alpha_B + (\frac{1}{2}\gamma_0^2+\frac{8}{3})\gamma_B + \frac{2}{3}\gamma_0^2\delta_B}{3\lambda_0 + 6\mu_0}. \tag{4.5}$$

Replacing the u's by the w^{∞}'s in Eq. (2.6), and making use of Eqs. (4.5), (2.12), (1.3b), (2.10b), and (2.10c), one obtains for the relaxation energy the expression

$$w_r = a^2\left(\frac{\Delta V^{\infty}}{\Omega}\right)\left(\frac{\sqrt{3}\gamma_0}{8\pi}(\beta_B' + 3\alpha_B + 4\gamma_B' + \frac{\delta_B}{\gamma_0}\right). \tag{4.6}$$

The results of the calculations of w^{∞}, $\Delta V^{\infty}/\Omega$, and W_r^{∞} are summarized in Tables III and IV. It may be remarked that in M1, one can express $\Delta V^{\infty}/\Omega$ and W_r^{∞} in terms of the elastic constants alone, by substituting for α_B and β_B [Eqs. (2.8d) and (2.8e) with $\gamma_B = 0$] in Eqs. (4.5) and (4.6). It must also be emphasized that for a finite elastic medium, image effect corrections ought to be made. As shown by Eshelby,[3] this has the effect of multiplying Λ, ΔV^{∞}, w^{∞}, and W_r^{∞} by a factor of $(3\lambda_0 + 6\mu_0)/(3\lambda_0 + 2\mu_0)$, which is equal to 1.659 for magnesium.

TABLE IV. Volume change ΔV^{∞} in units of Ω (=46.462 $\times 10^{-24}$ cm^3), and relaxation energy W_r^{∞} in eV.

	ΔV^{∞}	W_r^{∞}
$M1$	−0.0358	0.00136
$M2$	−0.0384	0.00147
$M3$	−0.1075	0.01360
$M4$	−0.0438	0.00275

V. DISCUSSION

The (perfect lattice) force constants which are used in our calculations in the various models are widely different (see Table I). However, the calculation of the dispersion all over the Brillouin zone does not differ significantly in the various models, besides reproducing reasonably well the observed dispersion at selected points. As a further check, we have computed also the perfect-crystal Green's-functions in M2, M3, and M4 (these results are not reported in this paper, as they are not directly relevant). Close agreement with the results quoted in Table II (which are based on M1 alone) is obtained. That the response of the lattice is rather insensitive to the choice of the lattice model has been mentioned previously by Tewary and Bullough[9] in the case of copper.

The situation is quite the contrary in the case of defect properties. This is clearly due to the fact that the defect is simulated by a set of "applied forces" which differ from model to model both quantitatively and qualitatively. For example, the forces on the first shell in M1 and M4 act inwards towards the vacancy, whereas they act outwards in M2 and M3. In the absence of a direct experimental measurement of E_r, it is not possible to conclude which particular model is the most appropriate one for defect calculations. Compared to the experimental value of the vacancy formation energy (values reported range from 0.58 to 0.89 eV),[10,11] our calculation yields a very small value for E_r. The approximate calculations (of W_r^{∞}) based on a combination of discrete and continuum models (M2, M3, and M4) lend further support to the smallness of this quantity. It should be mentioned that Doneghan and Heald, whose potential was used in M4, used a different method of calculation and reported $\Delta V = -0.13\ \Omega$ and $E_r = -0.13$ eV. Our approximate calculations (i.e., of ΔV^{∞} and W_r^{∞}) in M4 yield values for ΔV and E_r, respectively, that are smaller than the above values by factors of 3 and 48, approximately. Since the forces used in our calculations (in M4) are derived from the same potential that the above authors have used in their calculations, it is hard to believe that such large discrepancies can arise merely by the use of the defect forces $\{\vec{f}^*(n)\}$ instead of the perfect forces $\{\vec{f}(n)\}$. [Unfortunately the authors in Ref. 5 have not given the details of their calculations. For example, it is not clear how a "first guess" of ΔV (or E_r) was made.] It would

be interesting to extend the results of I (for the IR A_1' only) and perform defect-lattice calculations in M2, M3, and M4. Only such calculations would confirm or disprove the results of Doneghan and Heald[5] conclusively.

Note added in proof. Use of the proposed potential of Ref. 5 together with the calculated values of E_r (for M_1) and W_r (for $M2$, $M3$, and $M4$) yields for the vacancy formation energy the values (all in eV) 0.727 ($M1$), 0.715 ($M2$), 0.716 ($M3$), and 0.727 ($M4$). Results of the lattice calculations in the four neighbor extension of $M1$, $M2$, $M3$, and $M4$ have been forwarded for publication in Pramāna.

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