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ASYMPTOTIC ELASTIC ENERGY IN SIMPLE METALS*

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ABSTRACT

The asymptotic form of the elastic binding energy $\Delta E^{as}(R)$ between two Mg atoms in Al is expressed as a product of a lattice Green function and the dipole force tensor P. The quantity P is obtained by a nearly free electron model in which the impurity effect is introduced by a screened Ashcroft pseudopotential characterized by an excess charge ΔZ and a core radius r_j.

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I. INTRODUCTION

The interaction between two defects in a crystal can be separated into two main contributions: the first is a chemical term which takes place when the atoms are kept fixed to their original positions; the second is due to the atomic relaxation around the impurities and is called the elastic energy.

An attempt to estimate the elastic interaction between two impurities in a metal was firstly made using the elasticity theory[1,2]. In his approach, the author considers the components of the system as two spheres characterized by their atomic volumes and their elastic constants. Such a classical method describes well the asymptotic behaviour of the elastic energy which falls off as R^{-3} (R is the interdefect separation).

On the other hand a few authors[3,4,5] have considered the discrete nature of the lattice in which the normal expansion for atomic displacements is adopted. The introduction of an impurity into a substitutional or interstitial position in a pure metal causes displacements of atoms from their original positions and consequently the potential energy E of the system is changed. For small displacements, the variation of the potential energy δE, in the harmonic approximation, can be written as a Taylor series[6]:

$$\delta E = -\sum_{\lambda,\alpha} F_\alpha(\lambda)\, u_\alpha(\lambda) + \frac{1}{2}\sum_{\substack{\lambda,\alpha \\ \mu,\beta}} u_\alpha(\lambda)\; k_{\alpha\beta}(\lambda,\mu)\; u_\beta(\mu) \qquad (1)$$

where $u_\alpha(\lambda)$ is the displacement of the atom at λ in the direction α ($\alpha = x,y,z$). The force $F_\alpha(\lambda)$ acting on the metallic atom at site λ in the direction α is given by the first derivative of δE with respect to $u_\alpha(\lambda)$; the force constant $k_{\alpha\beta}(\lambda,\mu)$ is given by the second derivative (both derivatives are evaluated at the unrelaxed positions). If the force constant is assumed unchanged due to the defect[7]; then, for cubic crystals, the size effect $\frac{\Delta\Omega}{\Omega}$ is determined in terms of the dipole force tensor P and the elastic

constants of the solid C_{ij}, in the dilute limit we have

$$\frac{\Delta\Omega}{\Omega} = \frac{\mathrm{Tr}\, P}{(C_{11} + 2C_{12})} \qquad (2)$$

A simple expression is used to relate the force $F(\lambda)$ to the impurity screening charge[8].

$$F(\lambda) = Z_i\, \varepsilon(\lambda) \qquad (3)$$

where Z_i is the valency of the pure metal; $\varepsilon(\lambda)$ is the electric field induced by the screening charge and given by the gradient of the screened impurity potential. The dipole force tensor P is defined by the relation[9]:

$$P_{\alpha\beta} = \sum_{\lambda} \lambda_\alpha\, F_\beta(\lambda) \qquad (4)$$

(P for defects with cubic symmetry is diagonal i.e. $P_{\alpha\beta} = P\,\delta_{\alpha\beta}$).

In the following, we describe an estimate of the dipole force tensor P in normal metals using a pseudopotential model[10]. The notion of pseudopotential permits us to develop simple methods and to obtain good results but is only limited to small values of the impurity excess charge ΔZ[11]. That is why significant advances have been made in this domain. Some recent studies have used the pseudopotential theory to determine the size effect[12,13].

II. THE ELASTIC BINDING ENERGY

In the pseudopotential formulation for normal metals, it is possible to write the total energy of the system as contributions due to ions and electrons[14].

$$E = E_0 + E_e + E_{bs} \qquad (5)$$

E_0 is the energy of an atomic sphere of the metal, just a sphere of uniform electron gas with the ion at the center. E_e represents the Ewald interaction between point ions and a uniform compensating negative charge. E_{bs}, the band structure energy, is the ionic interaction via conduction electrons. The term E_0 can be neglected because of the smallness of the core size of our host metal (Al).

The additional normalized wave-number characteristic $\Delta\phi^N_{ij}(q)$ due to the defect is[10]:

$$\Delta\phi^N_{ij}(q) = \frac{1}{Z_i Z_j} \left| \frac{\Omega q^2}{4\pi} \right|^2 \omega_i^\circ(q)\, \Delta\omega^\circ(q) \left| 1 - \frac{1}{\epsilon(q)} \right| \qquad (6)$$

The indices i,j represent the host and impurity ions; $\epsilon(q)$ is the Hartree dielectric function. $\omega_i^0(q)$ is the bare ion pseudopotential form factor of the host lattice and has an Ashcroft analytic form:

$$\omega_i^\circ(q) = \frac{-4\pi Z_i}{\Omega q^2} \cos q r_i \qquad (7)$$

where r_i is the core radius of the atom i. For a substitutional alloy, the impurity form factor is presented by

$$\Delta\omega^\circ(q) = \omega_j^\circ(q) - \omega_i^\circ(q) \qquad (8)$$

A complete estimation of the dipole force tensor P in the free electron model and the nearly free electron model is found in (7) and (10) . Our major aim is to calculate the elastic interaction, $\delta E(R)$, between two magnesium atoms in an aluminium host; we have:

$$\Delta E(R) = \frac{1}{N} \sum_{q \in BZ} \sum_{\alpha,\beta} F_\alpha(q)\, G^L_{\alpha\beta}(q)\, F_\beta(q)\, e^{iq.R} \qquad (9)$$

where $G^L(q)$, $F(q)$ are the Fourier transforms of the static phonon Green function and the forces $F(\lambda)$ respectively. The summation over q is confined within the first Brillouin zone (BZ); N is the total number of

atoms in the crystal. In the long wave length limit (asymptotic approximation) we use the following expansion:

$$e^{-i\vec{q}\cdot\vec{\lambda}} \simeq 1 - i\vec{q}\cdot\vec{\lambda} \qquad (10)$$

From equation (4) we get

$$F_\alpha(\vec{q}) = -i \sum_\beta q_\beta P_{\beta\alpha} \qquad (11)$$

The asymptotic form of the elastic energy becomes

$$\Delta E^{as}(R) = -\sum_{\alpha,\beta} P_{\alpha\alpha} P_{\beta\beta} \frac{\Omega}{8\pi^3} \int d^3q \; G^L_{\alpha\beta}(\vec{q})\, q_\alpha q_\beta \, e^{i\vec{q}\cdot\vec{R}} \qquad (12)$$

where $P_{\alpha\alpha}$ is the α component of the dipole force tensor P. The lattice Green function $G^L_{\alpha\alpha}(q)$ is approximated by a phenomenological model[15] (i.e. given in terms of the elastic constants of AL and of the experimental values of the phonon energies) and replaced by its value of the elastic continuum.

Finally, $\Delta E^{as}(R)$ reduces to a one dimensional integral over the variable ϕ

$$\Delta E^{as}(R) = \frac{P^2\Omega}{8\pi^2 R^3} \int_0^{2\pi} d\phi \; f''(\hat{q}') \Big|_{\hat{q}\cdot\hat{R}=1} \qquad (13)$$

where $\hat{q}'$ is given in an appropriate coordinate system for $\hat{q}$ with respect to R. The function $f(\hat{q}')$ is written as

$$f(\hat{q}') = \sum_{\alpha,\beta} G^L_{\alpha\beta}(\vec{q}') \, q'_\alpha \, q'_\beta \qquad (14)$$

The second derivative $f''(\hat{q}')$ is calculated analytically whereas the simple integration over the variable ϕ is carried by Simpson rule (Table 1). The simplicity of the asymptotic interaction is due to the fact that we avoid the numerical difficulties such as the strong oscillations arising in the $e^{i\vec{q}\cdot\vec{R}}$ term by transforming the sum to a line integral[16,17].

III. CONCLUSION

In this work we have presented a formulation for the dipole force tensor P in terms of the screened potential. This quantity (P) of a substitutional Mg impurity in an Al host can be considered as a competition between two main contributions: the first is a charge dependence, which is directly proportional to the excess charge ΔZ, whereas the second depends on the core radii of the impurity and the host atoms. Our value of the dipole force tensor (TrP = 0.33 a.u.), compares favourably with other calculations using Shaw model pseudopotential[12], is injected in equation (13) so as to estimate the asymptotic elastic energy.

A comparison between the binding energies deduced from a free electron model[7] and the actual pseudopotential approach shows qualitative agreement for the few nearest neighbours (table 1), then the order of magnitude changes afterwards.

The above observation is due to the fact that in an isotropic medium $\Delta E^{as}(R)$ decreases as R^{-5} whereas in the pseudopotential model (anisotropic medium) the asymptotic elastic binding energy falls off as R^{-3}. Moreover, we have neglected in our description the modification of the force constants resulting from the presence of the foreign atom which has to be taken into account. This problem is presently under investigation.

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Table 1

Asymptotic elastic energy $\Delta E^{as}(R)$ (mev) between two magnesium atoms in an aluminium host with one Mg located at the origin and the other at a/2(h,k,l); a is the lattice parameter. The 1st column (2nd column) gives $\Delta E^{as}(R)$ for a free electron (pseudopotential) model.

h	k	l	$\Delta E^{as}(R)$ (mev)	
			Free Electron	Pseudopotential
1	1	0	3.425	5.041
2	0	0	-2.422	-5.009
2	1	1	0.220	0.618
2	2	0	0.107	0.630
3	1	0	-0.135	-0.806
2	2	2	0.104	0.789
3	2	1	0.026	0.202
4	0	0	-0.076	-0.626
3	3	0	0.014	0.186
4	1	1	-0.027	-0.312
4	2	0	-0.009	-0.119
3	3	2	0.020	0.273
4	2	2	0.007	0.077
4	3	1	0.006	0.090
5	1	0	-0.019	-0.261
5	2	1	-0.004	-0.093
4	4	0	0.003	0.078
4	3	3	0.007	0.144
5	3	0		-0.009
4	4	2	0.005	0.109
6	0	0	-0.010	-0.185
5	3	2	0.002	0.041
6	1	1	-0.006	-0.138
6	2	0	-0.004	-0.101

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