BINDING ENERGIES OF TRANSITION METAL IMPURITIES IN ALUMINIUM

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Binding energies of a vacancy and a transition metal impurity and those of two transition metal impurities at nearest neighbour distance in aluminium host have been calculated using the linear screening approximation and model potentials proposed by ANIMALU for transition metals.

Introduction

From the 1960's the pseudo or model potential technique has enjoyed widespread use in calculations of band structure, lattice dynamics, total energy, electrical transport properties of metals and interaction between point defects.

Recently TAKAI *et al.* [1—5] have performed calculations on binding energies of various impurity-vacancy complexes in aluminium using three kinds of exchange and correlation correction in the dielectric function for the screening, and Ashcroft's (empty core) pseudo potentials both for the simple metal impurities and for the aluminium host.

In this paper binding energies of a vacancy and a transition metal impurity and of those of two transition metal impurities at nearest neighbour distance in aluminium matrix are presented. In these calculations the linear screening approximation and, for the transition metal impurity, a model potential proposed by ANIMALU [6] have been used. With this potential, ANIMALU could reproduce the diverse features of the phonon spectra of some transition metals [7] and this fact encouraged us that the basic effects of the d-shell of the transition metal impurity are at least partly taken into account.

In this paper we shall briefly describe the effective interaction potentials and Animalu's model potential including the dielectric function and its correction factor. The results and discussion of our calculations on the vacancy-impurity and impurity-impurity binding energies in aluminium are presented.

Effectiv interaction between point defects

The interaction energy between two point defects at a distance r from each other can be expressed in the pseudo potential perturbation theory to second order, as [2]:

$$\Phi_{VV}(r) = \frac{Z_H^2 e^2}{r} + \frac{\Omega_H}{\pi^2} \int_0^\infty q^2 \frac{\sin qr}{qr} G_{HH}(q)\, dq,$$

$$\Phi_{VI}(r) = -\frac{Z_H \Delta Z_I e^2}{r} + \frac{\Omega_H}{\pi^2} \int_0^\infty q^2 \frac{\sin qr}{qr} [G_{HH}(q) - G_{HI}(q)], \tag{1}$$

$$\Phi_{IJ}(r) = \frac{\Delta Z_I \Delta Z_J e^2}{r} + \frac{\Omega_H}{\pi^2} \int_0^\infty q^2 \frac{\sin qr}{qr} [G_{HH}(q) - G_{IJ}(q) - G_{HI}(q) - G_{HJ}(q)]. \tag{2}$$

Here the indices H, V and I, J refer to the host, vacancy and impurities, respectively. In these expressions G_{ij} is the so-called energy-wave-number characteristic function defined by

$$G_{ij} = w_i(q) w_j(q) \varepsilon_H(q) \chi_H(q),$$

$$(i, j = H, V, I)$$

where $w_i(q)$ and $w_j(q)$ are the form factors of atom i and j, respectively. For aluminium we can use the Ashcroft's bare ion pseudo potential [8]:

$$v_H(q) = -\frac{4\pi Z e^2}{\Omega_H q^2} \cos(q \cdot R_c),$$

and the transition metal impurity can be described by Animalu's model potential

$$v(q) = B(q) + F(\vec{k}_F, \vec{k}_F + \vec{q}),$$

where $B(q)$ and $F(\vec{k}_F, \vec{k}_F + \vec{q})$ are defined in [6]. The form factor of an impurity atom is modified in screening and volume appropriate to the matrix. Namely [9] $w_I(q) = \Omega_I \varepsilon_I(q) w_I^0 / \Omega_H \varepsilon_H(q)$. The perturbation characteristic function $\chi_H(q)$ and dielectric

Table I

Impurities	Z_I	Ω_I (a. u.)	Binding energies (eV)			
			Vacancy-Impurity		Impurity-Impurity	
Cu	1	79.4	0.022	(−0.027)	0.046	(−0.027)
Ag	1	115.4	0.061	(−0.020)	0.020	(−0.015)
Au	1	114.6	0.181	(−0.027)	−0.247	(−0.027)
Zn	2	102.0	−0.047	(−0.007)	−0.025	(−0.001)
Hg	2	157.8	−0.018	(−0.019)	−0.022	(−0.016)

Binding energies in aluminium at nearest neighbour position. Also shown are the atomic volume Ω_I and the valences Z_I of the impurity atoms.

Table II

Impurities	Z_1	Ω_1(a. u.)	Binding energies (eV)	
			Vacancy-Impurity	Impurity-Impurity
Sc	3	168.7	−0.038	−0.019
Ti	4	119.0	−0.115	−0.024
V	5	93.9	−0.032	−0.051
Cr	3	80.6	−0.351	−0.286
Mn	2	81.9	−0.048	−0.022
Fe	3	79.8	−0.035	−0.016
Co	2	74.9	−0.080	−0.061
Ni	2	73.6	−0.081	−0.062
Y	3	223.1	0.076	−0.082
Zr	4	157.0	0.052	0.022
Nb	5	121.3	0.031	−0.002
Mo	6	105.5	0.082	−0.119
Tc	7	96.5	−0.052	0.192
Ru	4	91.9	0.118	−0.152
Rh	3	92.6	0.058	−0.048
Pd	2	99.3	−0.166	0.036
La	3	252.2	0.081	−0.072
Hf	4	150.2	0.060	0.005
Ta	5	121.3	0.028	−0.004
W	6	106.5	0.085	−0.096
Re	7	99.3	−0.024	0.149
Os	4	94.8	0.152	−0.172
Ir	4	95.5	0.151	−0.173
Pt	2	101.6	−0.124	0.016

Binding energies at nearest neighbour position in aluminium for 3d, 4d and 5d transition metal impurities.

function $\varepsilon_H(q)$ of a host metal are given by

$$\chi_H(q) = -\frac{1}{2}\frac{Z_H}{\frac{2}{3}\varepsilon_F}\left(\frac{1}{2}+\frac{4k_F^2-q^2}{8qk_F}\ln\left|\frac{2k_F+q}{2k_F-q}\right|\right),$$

$$\varepsilon_H(q) = 1-\frac{4\pi e^2}{\Omega_H q^2}(1-f(q))\chi_H(q).$$

Here

$$f(q) = A\{1-\exp[-B(q/k_F)^2]\}$$

is the SSTL approximation for the correlation and exchange effects, with $A=0.9048$ and $B=0.3363$ for aluminium [10].

Results and discussion

Using equations (1)—(2) and potential parameteres in Table I of reference [6], binding energies have been calculated and the results for Cu, Ag, Au, Zn and Hg are presented in Table I. In order to estimate the effects of using Animalu type potential instead of Ashcroft's type the results of TAKAI AT AL [5] are also given (figures in parantheses). For aluminium, the Ashcroft's potential with $Z_{Al}=3$ and $R_c=1.12$ a.u. was used both by TAKAI ET AL. and in the present work.

In Table II binding energies for the 3d, 4d and 5d transition metals are listed. The present calculation is based on the second-order perturbation theory using pseudopotential formulation. It is well-known that this approach can be appropriate only for impurities with small ΔZ_I, that is only for the first two or three members of the transition metal series. On the other hand, the lattice distortion caused by impurities has been completely neglected which, however, can play an important role, especially when the size of the impurity is considerably different from that the host.

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ЭНЕРГИИ СВЯЗИ ПРИМЕСНЫХ ПЕРЕХОДНЫХ МЕТАЛЛОВ В АЛЮМИНИИ

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Рассчитаны энергии связи вакансии, примесного переходного металла и двух примесных переходных металлов в ближайшем соседстве расположенных в алюминии. Использованы приближение линейного экранирования и модельный потенциал, предложенный Анимали для переходных металлов.