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Study of driving forces for atomic migration in metals and dilute alloys

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We present a pseudopotential calculation of the driving forces for atomic migration in the metals and dilute alloys in the presence of electron currents. The forces on an atom arising from the applied electric field and from the electron scattering together comprise the driving force, causes a net current of atoms. A well recognized Ashcroft's empty core (EMC) local model potential is used to investigate the driving forces for interstitial F_{INT} and vacancy F_{VAC} migration in several metals and their dilute alloys. The present study concludes that F_{INT} is larger than $F_{VAC.}$ For some dilute alloys the electron scattering force is found in the opposite direction to the electron drift velocity. Present findings are compared with the other such data, which confirms the applicability of the model potential.

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1. Introduction

The application of an electric field to a metal gives rise to a current of electrons and to a considerably smaller current of atoms. The migration of atoms in a metal, which is subjected to an electric field, is the phenomenon known as electromigration. From a fundamental point of view the study of electromigration is interesting because it involves microscopic electric fields and subtle dynamical processes occurring into coupled electron and atom transport from a technological point of view electromigration is important because it is a major failure mechanism in an operation of solid-state electronic devices. Circuit failure due to electromigration damage is of increasing concern to the semiconductor industry; it pushes in exorably toward further miniaturization of integrated circuits. It is also important for the purification of materials. Hence we thought it worthwhile to undertake the investigation of electromigration driving forces in certain metals and their dilute alloys. In general, the electromigration driving force consists of two contributions. One contribution is called the electrostatic force and is the force from applied electric field. The second contribution is called the electron scattering force and is the force arises from the scattering of electrons by the atom or ion [1-3].

A pseudopotential based theory of the driving forces for electromigration in metals was developed by Sorbello [1-3] in the past. Recently theory of electromigration is modified by Lodder [4,5]. From the literature survey it is found that, nobody can perform this type of computation of the driving forces in the recent years with the help of model potential formalism. Hence, in the present paper, we thought it worthwhile to under take the investigation of the driving forces for atomic migration in some metals and dilute alloys.

The pseudopotential picture is adopted for the computation of electron scattering force **F**. The model potential used in the present study is [6],

$$V(q) = \frac{-8\pi Z}{\Omega_O q^2 \varepsilon(q)} \cos(q r_C), \quad (1)$$

where Z is the valency, Ω_0 the atomic volume, q the wave vector, r_C the parameter of the model potential and $\varepsilon(q)$ is the static Hartree dielectric function [7].

2. Computational methodology

Within a pseudoatom picture of a metal we can consider the ions in the absence of a field to be locally neutral objects resembling atoms, called "pseudoatoms" [7]. By adopting pseudopotential theory, the electron scattering force on the j^{th} pseudoatom assumed to be at position $\mathbf{r_j}$, is given by [1-3]

$$F_j = -2\pi \sum q\, w_j(q)\, w_i(q)\, f_k \exp[i q \cdot (\mathbf{r}_i - \mathbf{r}_j)] \delta(\epsilon_k - \epsilon_{k+q}), \quad (2)$$

where the sum is over **k** and **q** and over all the atoms in the crystal, $f_{\mathbf{k}}$ is the perturbed Fermi-distribution in the presence of the **E** and w_j is the pseudopotential of the j^{th} ion.

The electron scattering force on an ion is given by the negative gradient of the effective potential, which involves two-body effective interaction between the ion and all defects. To calculate the electromigration driving forces, we have considered diffusion to occur via the interstitial or vacancy mechanisms, and we define these forces to be positive if they are in the same direction as drift velocity $\mathbf{v}_d$, and negative if in the opposite direction. We proceed first to pure metals and afterwards to the dilute alloys.

2.1 Pure metals

2.1.1 Interstitial diffusion

The diffusion of interstitial atoms consists of the jump of an atom between two interstitial positions. By ignoring distortions of the crystal during the jump, the driving force for electromigration, F_{INT}, is [1-3],

$$F_{INT} = \frac{\Omega_0^2 m k_F}{12\pi^3\hbar^2}\left(\frac{v_d}{v_F}\right)\int_0^{2k_F} w(q)^2 q^3 dq, \qquad (3)$$

here m is the mass of electron, v_F the Fermi velocity, v_d the electron drift velocity and k_F the Fermi wave vector, respectively.

2.1.2. Vacancy diffusion

In this mechanism, an atom undergoes a diffusion jump from a regular lattice site to a neighboring vacancy. The driving force in this mechanism is the average of the actual force over the jump path ℓ and the expression of F_{VAC} is [1-3],

$$F_{VAC} = -\frac{\Omega_0^2 m k_F}{4\pi^3\hbar^2}\left(\frac{v_d}{v_F}\right)\left\{\frac{2}{\ell}\int_0^{2k_F} w(q)^2 q^2 j_1(q\ell)\, dq - \frac{1}{3}\int_0^{2k_F} w(q)^2 q^3 dq\right\}, \qquad (4)$$

where $j_1(q\ell)$ is the spherical Bessel function.

2.2 Dilute alloys

Since we are considering a very dilute alloy we shall consider the impurity atom to be surrounded by host atoms. To perform the calculations we define w′(q) to be the form factor of the foreign impurity species and multiply by Ω_0'/Ω_0, where Ω_0' is the atomic volume of the impurity species. Also, w(q) must be replaced by w′(q) in equation (3) for interstitial diffusion. For vacancy diffusion, $w(q)^2$ must be replaced by w (q) w′(q) in the first integral, and by $w'(q)^2$ in the second integral of equation (4).

2.2.1 Substitutional diffusion

In interstitially mechanism, the impurity jumps from a lattice site to an interstitial position. By taking the defect to be a host vacancy and a foreign impurity at the same lattice site, the force on a substitutional impurity is [1-3],

$$F_{SUB} = \frac{\Omega_0^2 m k_F}{12\pi^3\hbar^2}\left(\frac{v_d}{v_F}\right)\int_0^{2k_F} w'(q)[\, w'(q) - w(q)\,] q^3 dq \qquad (6)$$

Where n is electron concentration of the metals and dilute alloys, respectively.

3. Results and discussion

The input parameters and other constants used in the present computation of the driving forces in metals and dilute alloys are narrated in Table 1. The present results regarding the electromigration driving forces in 9 metals and 16 dilute alloys are tabulated in Tables 2 and 3. The results are comparable and compatible with such other theoretical results [1-3]. From the Table 2, it is noted that the results of F_{INT} and F_{VAC} are found qualitative agreement with the theoretical data of Sorbello [1-3]. Also the values of both forces for Cu, Ag and Au of Sorbello [1-3] are found very different from our results. The computed data of the F_{INT}, F_{VAC} and F_{SUB} are narrated in the Table 3. Here also same trends are observed in the case of 16 dilute alloys. The present results are fond qualitative agreement with the theoretical data [1-3]. The results displayed in Tables 1 and 2 indicate that the calculations are sensitive to choice of the form factor. However, similar trends are found in our and in Sorbello's [1-3] calculations. That is discrepancies found in the computation of F_{INT} and F_{VAC} around 0.52 – 62.99% and 4.44 – 61.20% often occur in the present results obtained with EMC model potential with the Sorbello's data [1-3] for the same systems in the case of metals. Large discrepancies are found in the case of noble metals around 51.70 – 62.99%. To obtain more reliable results one should abandon the local potential approach used here to construct the form factors w(q). While these discrepancies found in the results of F_{INT} and F_{VAC} are 0.13 – 60.74%, 0.02 – 85.74%. Very large discrepancies are found in the results of F_{SUB}. Also from Tables 2 and 3, it is noted that F_{INT} is greater than F_{VAC} because an ion that moves between two vacant sites experiences the fields of individual dipoles centered at each vacant site and these vacancy dipoles are oriented opposite to the dipole carried by the moving ion. Also the value of F_{SUB} for some dilute alloy is negative because substitutional impurity may feel an electron scattering force opposite to the electron drift.

Table 1. Input parameters and other constants.

Metal	Z	Ω_0 (au)	r_C (au)	$v_F \times 10^8$ (cm/s)	$n \times 10^{22}$ (cm^{-3})	ℓ (au)
Li	1	144.9	3.12	1.29	4.70	3.023
Na	1	254.5	2.62	1.07	2.65	3.659
K	1	481.4	3.33	0.86	1.40	4.525
Cu	1	79.7	1.26	1.57	8.45	2.560
Ag	1	115.1	1.62	1.39	5.85	2.890
Au	1	114.4	1.27	1.39	5.90	2.880
Mg	2	155.9	2.17	1.58	8.60	3.200
Cd	2	144.8	1.92	1.62	9.28	2.980
Al	3	111.3	1.81	2.02	18.10	2.860

Table 2. Electron scattering forces in metals (eV/cm).

Metal	F_{INT} x [10^6/j(A/cm^2)]		F_{VAC} x [10^6/j(A/cm^2)]	
	Present	[1-3]	Present	[1-3]
Li	51.75	58	37.99	31
Na	82.71	77	42.92	37
K	105.95	103	50.63	53
Cu	96.25	246	76.04	196
Ag	92.16	249	68.45	171
Au	144.89	300	119.02	229
Mg	114.59	114	78.83	71
Cd	125.11	144	79.48	110
Al	165.87	158	116.97	112

Table 3. Electron scattering forces x [10^6/ j (A/cm^2)] in eV/cm on solute atoms of dilute alloys.

Host	Impurity	F_{INT}		F_{VAC}		F_{SUB}	
		Present	[1-3]	Present	[1-3]	Present	[1-3]
Li	Na	95.98	93	61.34	55	72.08	34
	K	152.90	-	116.51	-	116.12	-
Na	Li	46.33	49	16.29	17	21.21	-1
	K	129.37	128	77.32	77	26.22	29
K	Li	32.27	-	7.97	-	8.55	-
	Na	66.38	63	22.26	21	-16.98	-17
Cu	Mg	113.28	113	65.01	35	55.26	-53
	Cd	129.70	139	74.23	58	37.36	-58
Ag	Li	58.71	63	26.21	17	50.51	-55
	Mg	105.08	100	51.76	30	42.01	-47
Au	Li	57.22	63	24.18	19	62.91	-68
	Ag	98.14	250	63.20	174	-21.63	-21
Mg	Li	66.97	72	38.40	43	-8.90	-15
	Al	126.88	123	81.12	75	8.65	7
Al	Mg	146.19	146	106.11	107	-5.42	-2
	Zn	142.63	144	111.03	111	32.08	1

4. Conclusions

From the present study, it is concluded that the model pseudopotential theory is able to generate the consistent results of the driving forces in atomic migrations in metals and dilute alloys. The calculated forces are in reasonable agreement with the reported data. Also, the numerical results are rather sensitive to the proper choice of form factor. F_{INT} is found greater than the F_{VAC} in most of the metals and dilute alloys. Such study on atomic migration force in other metals and dilute alloys is in progress.

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