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Atomic mobilities and diffusivities in U-X (X = Nb, Zr, Ti) bcc alloys

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ABSTRACT

Based on a critical evaluation of experimental diffusion data available in the literature and the updated thermodynamic descriptions within the CALPHAD framework, the atomic mobilities of U, Nb, Ti, and Zr in U-X (X = Nb, Zr, Ti) bcc alloys were assessed with the DICTRA software. For each system, comprehensive comparison shows that a good agreement between the calculated and experimental data was obtained. The developed mobilities in conjunction with the thermodynamic parameters were also used to describe the marker movement in the U/Zr as well as U/Ti diffusion couples, and a satisfactory result was obtained. The presently obtained atomic mobilities can describe diffusion phenomenon more accurately than previously reported atomic mobilities.

1. Introduction

Uranium-based alloys used as nuclear fuel materials have gained great technological interests due to their high strength, ductility, and good oxidation and radiation resistances. Ti, Nb, and Zr have been proved to be promising alloying elements in advanced U-based alloy. For instance, the addition of Ti is beneficial to increasing the strength and toughness of uranium alloys, and Nb is characterized by excellent high temperature corrosion resistance [1,2], and the addition of Zr improves the thermal conductivity, burn-up capability and the solidus temperature [3,4]. Besides, the stability of the body-centered cubic phase is promoted by summating a variety of alloying elements with bcc lattice, such as Nb and Ti, which greatly reduces the possibility of radiation swelling due to the decomposition of the bcc phase in Uranium-based alloys [5].

Most solid-state reactions are largely dependent upon thermodynamic behavior and complex diffusion processes. Practically, a good knowledge of diffusion information is needed to establish process flow sheets for fabrication and the service life prediction of alloys [6,7]. Therefore, it is of great interest to develop reliable thermodynamic and kinetic databases for U-based alloys, so as to get an insight into the diffusion-controlled transformation and facilitate new alloy design. Although the thermodynamic studies for U-based alloys are reported in the literature [8–10], a relatively less attention has been paid to the development of the kinetic database.

This work aims to assess the atomic mobilities for bcc phase of U-X (X = Nb, Ti, Zr) binary systems, including: 1) critically evaluating diffusion data available in the literature in the aspects of both experiments and calculations; 2) establishing a new set of self-consistent mobility database for these bcc phases using the CALPHAD method based on the updated thermodynamic database.

2. Model description

The temporal and spatial evolution of the diffusing species k in an n-component system can be generally described by Fick's law in the mass conservation form as follows:

$$\frac{\partial Ck}{\partial t} = \nabla Jk \quad (k = 1, \ \ldots, \ n) \tag{1}$$

where C_k is the concentration of element k with the unit of moles per volume; t is time; ∇ denotes the divergence operator. In a volume-fixed frame of reference, the flux J_k of species k follows Fick's first law, which is expressed as follows:

$$Jk = -\sum_{j=1}^{n-1} \widetilde{D}_{kj}^{n} \nabla Cj \tag{2}$$

where $\widetilde{D}_{kj}^{n}$ denotes the interdiffusion coefficient. $\widetilde{D}_{kj}^{n}$ in a substitutional solution phase can be given by the following expression [11]:

$$\widetilde{D}_{kj}^{n} = \sum_{i} (\delta_{ik} - x_k) x_i M_i \left(\frac{\partial \mu_i}{\partial x_j} - \frac{\partial \mu_i}{\partial x_n}\right) \tag{3}$$

where δ_{ik} is the Kronecker delta ($\delta_{ik} = 1$ if $i = k$, otherwise $\delta_{ik} = 0$); x_i

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Table 1
Experimental diffusion data in bcc_A2 U-Nb, U-Zr and U-Ti alloys.

Diffusion data type		Method	Temperature (K)	Composition range	Year	Ref	Code[#]
Impurity diffusion coefficient	D_U^{Nb}	SS	1923-2273	100 at. % Nb	1971	[23]	■
	D_U^{Zr}	SS	1173-1873	100 at. % Zr			
	D_U^{Nb}, D_{Nb}^U	SS	1250-1673	100 at. % Nb	1962	[21]	■
	D_U^{Nb}	LS	1773-2273	100 at. % Nb	1965	[24]	□
	D_{Nb}^U	LS	1064-1375	100 at. % Nb	1964	[26]	□
	D_{Nb}^U	DC	1073-1269	100 at. % Nb	1960	[25]	■
Interdiffusion coefficient	$\widetilde{D}_{NbNb}^U$	SS	1353	0-100 at. % Nb	1984	[27]	■
	$\widetilde{D}_{TiTi}^U$	DC	1223-1348	5-90 at. % U	1960	[38]	■
	$\widetilde{D}_{ZrZr}^U$	DC	1223-1348	10–95 at. % Zr	1956	[30]	■
		DC	1223-1723	15 at. % U	1968	[31]	■
		DC	973-1223	10–95 at. % Zr	1996	[32]	■
		DC	1223-1358	100 at. % U	1997	[33]	■
		DC	1223-1338	12.5-100 at. % Zr	1960	[34]	■
		DC	973-1023	68-75at. % Zr	1998	[35]	□
Tracer diffusion coefficient	D_U^*	DC	1073-1313	10 at. % U	1959	[20]	■
	D_U^*	LS	1173-1873	100 at. % Zr	1971	[23]	■
	D_U^*, D_{Nb}^*	TST	1203-2173	5-90 at. % Nb	1972	[22]	■
	D_U^*	SS	1188-1298	100 at. % Ti	1966	[31]	■
	D_U^*	SS	1188-1473	100 at. % Ti	1967	[36]	■
	D_U^*	–	1182-1775	100 at. % Ti	1978	[37]	■
	D_U^*, D_{Zr}^*	LS	1073-1338	100 at. % U	1968	[29]	■

[#] Indicates whether the data are used or not used in the atomic mobility assessment: ■, used; □, not used;
*LS denotes lathe sectioning technique, TST denotes the thin-layer sectioning technique, SS denotes the serial sectioning technique, DC denotes the diffusion couple, using the Matano method [28] to analyse, – denotes not reported.

Table 2
Summary of the atomic mobilities of U, Nb,Ti and Zr in bcc_A2 U-X alloys (X= Nb,Ti,Zr) (all in SI units).

Mobility	Parameters	Reference
Mobility of U	$\Phi_U^{U:Va} = -12127.11 - 132.24*T$	[16]
	$\Phi_U^{Nb:Va} = -325573.8357 - 174.7884*T$	This work
	${}^0\Phi_U^{Nb,U:Va} = +58942.86458$	This work
	${}^1\Phi_U^{Nb,U:Va} = 53739.0811 - 79.31080532*T$	This work
	$\Phi_U^{Zr:Va} = -63339.8623 - 185.886518*T;\ T \le 1528$ $= -136978.033 - 137.342172*T;\ T \ge 1528$	This work
	${}^0\Phi_U^{Zr,U:Va} = -57818.48602 - 14.5320922*T$	This work
	${}^1\Phi_U^{Zr,U,Va} = 306176.3524 - 217.0068316*T$	This work
	${}^2\Phi_U^{Zr,U:Va} = -331919.7894 + 221.1394667*T$	This work
	${}^3\Phi_U^{Zr,U:Va} = 259941.2167 - 81.41755759*T$	This work
	$\Phi_U^{Ti:Va} = -130395.607 - 133.1624*T$	This work
	${}^0\Phi_U^{Ti,U:Va} = -67672.8618$	This work
	${}^1\Phi_U^{Ti,U:Va} = -90161.4419$	This work
Mobility of Nb	$\Phi_{Nb}^{Nb:Va} = -395598.95 - 82.03*T$	[15]
	${}^0\Phi_{Nb}^{U:Va} = -142727.3035 - 147.8593*T$	This work
	${}^0\Phi_{Nb}^{Nb,U:Va} = -131116.1954 + 32.8683*T$	This work
	${}^1\Phi_{Nb}^{Nb,U:Va} = +87600.83654$	This work
Mobility of Zr	$\Phi_{Zr}^{Zr:Va} = -104624.81-163.15*T;\ T \le 1573$ $= -161543.53-126.10*T;\ T \ge 1573$	[15]
	$\Phi_{Zr}^{U:Va} = -68401.2748 - 206.169881*T$	This work
	${}^0\Phi_{Zr}^{Zr,U:Va} = -279055.1348 + 35.5309*T$	This work
	${}^1\Phi_{Zr}^{Zr,U:Va} = -64253.48703 + 25.3993*T$	This work
	${}^2\Phi_{Zr}^{Zr,U:Va} = -43464.92562 + 44.9128*T$	This work
	${}^3\Phi_{Zr}^{Zr,U:Va} = -50050 - 200.2*T$	This work
Mobility of Ti	$\Phi_{Ti}^{Ti:Va} = -151989.95 - 127.37*T$	[18]
	$\Phi_{Ti}^{U:Va} = -117814.875 - 137.6728*T$	This work
	${}^0\Phi_{Ti}^{Ti,U:Va} = -934004.47$	This work
	${}^1\Phi_{Ti}^{Ti,U:Va} = -928143.395$	This work

*Temperature(symbolized T) in Kelvin.

and μ_i are the mole fraction and the chemical potential of element i, respectively; n, k and j are the dependent, diffusing and gradient elements, respectively; M_i is the composition -dependent atomic mobility for element i.

According to the absolute rate theory, the mobility of element i can be divided into a frequency factor M_i^0 and an activation enthalpy Q_i [12]:

$$M_i = \exp(\frac{RT\ln(M_i^0)}{RT})\exp(\frac{-Q_i}{RT})\frac{1}{RT}{}^{mg}\Omega \quad = \frac{1}{RT}\exp(\frac{\Phi_i}{RT}) \tag{4}$$

where R is the gas constant; T is the absolute temperature; ${}^{mg}\Omega$ is a factor taking into account the effect of the ferromagnetic transition the magnetic factor on the mobility [13]. In the spirit of the CALPHAD framework, Φ_i depends on the composition and temperature, expressed by the Redlich–Kister polynomials [14] as below:

$$\Phi_i = \sum_j x_j \Phi_i^j + \sum_j \sum_{k>j} x_j x_k \left[\sum_{r=0,1,2...n} {}^r\Phi_i^{j,k}(x_j - x_k)^r \right] \tag{5}$$

where x_j and x_k are the mole fraction of element j and k respectively; Φ_i^j is the value of Φ_i for i in pure j, as for either self-diffusion ($i = j$) or impurity diffusion($i \ddagger j$); ${}^r\Phi_i^{j,k}$ is the interaction term for diffusion between U and element X (X = Nb, Ti or Zr).

Assuming a mono-vacancy atomic exchange mechanism for diffusion and neglecting correlation factors, the tracer diffusion coefficients of element i can be related to the atomic mobility via the Einstein relation:

$$D_i^* = RTM_i \tag{6}$$

In the A-B binary system, the interdiffusion coefficient $\widetilde{D}$ is expressed by the Darken equation:

$$\widetilde{D} = (x_A D_B^I + x_B D_A^I) = (x_A D_B^* + x_B D_A^*)\varphi \tag{7}$$

where D_A^I and D_B^I are the intrinsic diffusion coefficients of components A and B, respectively; D_A^* and D_B^* are the tracer diffusion coefficients of components A and B, respectively; φ is the thermodynamic factor, and it can be written as:

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