First principles calculations of alloying element diffusion coefficients in Ni using the five-frequency model*

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The diffusion coefficients of several alloying elements (Al, Mo, Co, Ta, Ru, W, Cr, Re) in Ni are directly calculated using the five-frequency model and the first principles density functional theory. The correlation factors provided by the five-frequency model are explicitly calculated. The calculated diffusion coefficients show their excellent agreement with the available experimental data. Both the diffusion pre-factor (D_0) and the activation energy (Q) of impurity diffusion are obtained. The diffusion coefficients above 700 K are sorted in the following order: $D_{\rm Al} > D_{\rm Cr} > D_{\rm Co} > D_{\rm Ta} > D_{\rm Mo} > D_{\rm Ru} > D_{\rm W} > D_{\rm Re}$. It is found that there is a positive correlation between the atomic radius of the solute and the jump energy of Ni that results in the rotation of the solute-vacancy pair (E_1). The value of E_2–E_1 (E_2 is the solute diffusion energy) and the correlation factor each also show a positive correlation. The larger atoms in the same series have lower diffusion activation energies and faster diffusion coefficients.

Keywords: first-principles theory, diffusion coefficients, alloying element, superalloy, activation energy and diffusion pre-factor

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1. Introduction

The superalloy displays excellent mechanical properties and oxidation resistance at elevated temperatures. Nickel, which exhibits a stable FCC (face-centred cubic) crystal structure from room temperature to its melting point,[1] is chosen as the solvent for the Ni-based superalloys.[2] The diffusion-related phenomena have become an increasingly important consideration during both processing and usage of the superalloys.[3] In the solidification process of single crystal superalloy, the dendrites grow at a rate which is greatly controlled by the solute diffusion.[4] In the heat-treatment process, atomic diffusion becomes accelerated in order to generate the microstructure, which is stable during operations over a prolonged period. During the service, the creep strain rate is proportional to the diffusion coefficient.[5] The formation of topological close packed (TCP) phases over a long-period service is associated with the diffusion process. The rafting of γ' is another important example of diffusion assisted coarsening.[6] Diffusion also affects the surface stability, and oxidation occurs at a rate that is diffusion-controlled.[7] Coatings are performed to protect the superalloys, the interdiffusion between the coatings and superalloy occurs during operation, leaving a degraded coating and a change of structure of the substrate.[8] Clearly, the diffusion process is important for investigating how to obtain the best properties of superalloys.

In recent years, the solute atom diffusivities were calculated by the density-functional theory (DFT) in a binary system.[9–14] The diffusion system includes the BCC (body-centred cubic) (α-Fe),[9] FCC,[10–12] and HCP (hexagonal close-packed)[14] structures. Kremar *et al.*[10] and Janotti *et al.*[12] exhibited the diffusion coefficients of transition elements in FCC Ni via first principles calculations. However, the formula of calculating the correlation factors in Refs. [10] and [12] was different from those of calculating FCC structures,[11,15,16] and the pre-factors were not explicitly calculated, so the calculated diffusion coefficients of 3d transition metal solutes in nickel[10] deviated from the experimental results.

In the present investigation, the diffusion coefficients of alloying elements (Al, Mo, Co, Ta, Ru, W, Cr, Re) in Ni are calculated using the five-frequency model and the first principles calculations. The purpose of the present study is to evaluate the diffusion

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coefficients of the alloying elements in Ni, and hopefully to make sense of what factors affect the diffusion rate, to give a further physical explanation of the alloying mechanism of alloying elements in superalloys.

2. Theory and computational approach

The diffusion in FCC metal occurs predominantly by a vacancy mechanism at medium and high temperatures. Mono-vacancies dominate the diffusion process at temperatures of $T \leq 2/3T_{\rm m}$ ($T_{\rm m}$ is the melting point of the metal). Additonally, the contributions of di-vacancies are also as significant as mono-vacancies at high temperatures of $T \geq 2/3T_{\rm m}$.[16,17] Le Claire[18−20] described the classic "five-frequency formula" of the vacancy mechanism for impurity diffusion in the FCC metal, which includes only the effect of mono-vacancies. The formula to calculate the effect of di-vacancies, developed by Mehrer,[17] is similar to the "five-frequency formula".

Figure 1 illustrates the five-frequency model for the vacancy jumps in a FCC crystal near an impurity.[11,16] In the figure, w_0 is the host atom jump without an impurity; w_1 is the jump of the host atom that results in the rotation of the solute-vacancy pair; w_2 is the solute atom jump; w_3 is the host atom jump that dissociates the solute-vacancy jump; w_4 is the reverse jump of w_3. The five-frequency formula gives the ratio of solute diffusion to the solvent self-diffusion by a vacancy mechanism, described as[11,16]

$$\frac{D_{\rm s}}{D_0} = \frac{f_2}{f_0}\frac{w_2}{w_1}\frac{w_4}{w_0}\frac{w_1}{w_3}. \tag{1}$$

Here, $D_{\rm s}$ is the solute diffusion rate; D_0 is the self-diffusion rate of the pure host atom; f_2 is the correlation factor for impurity diffusion; f_0 is the self-diffusion factor; w_x ($x = 0 \sim 4$) are the atom jump frequencies as illustrated in Fig 1. Three types of w_3 and w_4 are possible in the FCC lattice. $w_{3{\rm a}(4{\rm a})}$, $w_{3{\rm b}(4{\rm b})}$, and $w_{3{\rm c}(4{\rm c})}$ correspond to the second, third, and fourth nearest neighbouring site to the impurity respectively. The activation energies for the three w_3's were found to be identical within 0.02 eV, and the three w_4 jumps have the same results.[16] The values of $w_{3{\rm c}}$ and $w_{4{\rm c}}$ were considered, as the fourth nearest neighbouring positions are most similar to the bulk positions. The self-diffusion rate of the host atom can be determined through[11,21]

$$D_0 = f_0 w_0 a^2 \exp\left(-\frac{\Delta G_{\rm f}^0}{k_{\rm B}T}\right), \tag{2}$$

where a is the lattice parameter of the FCC host; $\Delta G_{\rm f}^0$ is the vacancy formation energy of the pure host system; $k_{\rm B}$ is the Boltzmann constant and T is the temperature.

The correlation factor f_2 is obtained via the following equations:

$$f_2 = \frac{2 + 7(w_3/w_1)F(w_4/w_0)}{2 + 2(w_2/w_1) + 7(w_3/w_1)F(w_4/w_0)}, \tag{3}$$

where

$$F(x) = 1 - \frac{1}{7}\frac{10x^4 + 180.5x^3 + 927x^2 + 1341}{2x^4 + 40.2x^3 + 254x^2 + 597x + 435} \tag{4}$$

with $x = w_4/w_0$.

Krcmar *et al.*[10] and Janotti *et al.*[12] assumed in their work that $F(x) = 1$, which means $w_4 \gg w_0$. However, our calculation is not based on the assumption that $w_4 \gg w_0$. When the solute is Ni, the same as the solvent, there is $w_0 = w_1 = w_2 = w_3 = w_4$, so $F(1) = 0.7356$ and $f_0 = 0.781$.

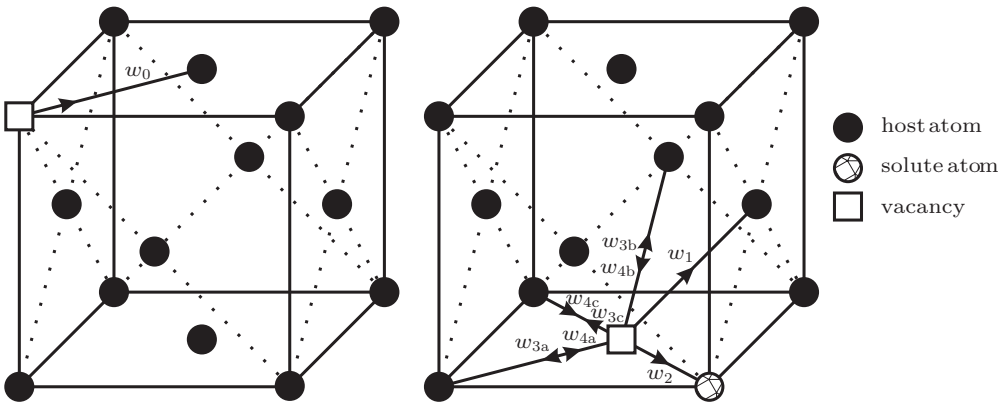


Fig. 1. The five-frequency model illustrating the vacancy jumps in FCC crystal near an impurity.

The jump frequency is written as that given by an Arrhenius expression based on the transition state theory (TST),[11,16] that is,

$$w_i = v_i \exp\left(-\frac{\Delta H_{\rm m}}{kT}\right) = v_i \exp\left(-\frac{E_i - S_i T}{kT}\right), \quad (5)$$

where v_i is the vibrational frequency; $\Delta H_{\rm m}$ is the change of enthalpy between the states when the diffusing atom is in its initial stable state and at the saddle point; E_i is the activation energy; S_i is the activation entropy. The vibrational frequencies of the host atoms vary little, so we assume that $v_0 = v_1 = v_3 = v_4$. The vibration frequency of the impurity atom can be approximated by[15,16,22]

$$\frac{v_2}{v_0} = \sqrt{\frac{m_0 T_{\rm m2}}{m_2 T_{\rm m0}}}, \quad (6)$$

where $T_{\rm m2}$ and $T_{\rm m0}$ are the melting points (in Kelvin) of the impurity and the host; m_0 and m_2 are the atomic masses of the host and impurity, respectively.

We also assume $S_0 = S_1 = S_3 = S_4$, because the activation entropies vary little,[16] and

$$S_2 = S_0 + \frac{\beta(E_2 - E_1)}{T_{\rm m0}}, \quad (7)$$

where $\beta = 0.4$, w_4 is the reverse jump of w_3 and hence, these two jumps have the same transition states, so

$$\frac{w_4}{w_3} = \exp\left(-\frac{\Delta G_{\rm b}}{k_{\rm B} T}\right), \quad (8)$$

when $\Delta G_{\rm b} = E_3 - E_4$. Here, $\Delta G_{\rm b}$ represents the energy change between the final state of w_4 and initial state of w_4.

Given the above information, only the activation energies (E_i, $i = 0 \sim 4$), and w_0 need to be calculated.

All the calculations are performed with the Vienna *ab initio* simulation package (VASP, version 4.6)[23,24] based on the plan-wave pseudo potential DFT[25,26] within the generalized gradient approximation (GGA).[27] We solve the density-functional equations with the ultra-soft pseudo potential method[23] and the Perdew–Wang parameterization (PW91) as well.[28,29] A supercell consisting of 32 lattice sites (2×2×2 cubic representation), with one host atom replaced by an impurity atom, is used in this study. A convergence test indicates that an energy cut-off of 400 eV and a Monkhost–Pack k-point mesh of 6×6×6 can yield an energy within 0.02 eV. The self-consistent convergence of the total energy is at 1×10^{-4} eV and the maximum force on the atoms is within 0.01 eV/A. The magnetism is applied to the system since Ni has a strong magnetism.

Diffusion barrier energy ($E_{\rm b}$) is obtained as the total energy difference between the solute atom at the saddle point and that at the initial stable point. The energy of the saddle point is calculated by fixing the solute atom position, and the host atoms are fully relaxed.

The vacancy formation energies in a pure Ni system ($E_{\rm f}^{\rm V(Ni)}$) are obtained by

$$E_{\rm f}^{\rm V(Ni)} = E(N-1,1,V_{N-1}) - \frac{N-1}{N} E(N,0,V_N) + B\Delta V. \quad (9)$$

Here, $E(N,x,V)$ denotes the energy of the system with N atoms and x vacancies occupying $N+x$ lattice sites in volume V; B is the bulk modulus of the Ni system, which is 188 GPa calculated in this study; ΔV is the volume change per atom with

$$\Delta V = \frac{V_{N-1}}{N-1} - \frac{V_N}{N}.$$

In a very large system ($N \to \infty$), $\Delta V \to 0$, the $B\Delta V$ can be neglected. The $B\Delta V$ contributes a lot to the total energy change because a comparably simple supercell (with 32 lattice sites) is used in this study.

The solute-vacancy binding energy ($E_{\rm f}^{\rm s-v}$) is calculated by

$$E_{\rm f}^{\rm s-v} = E(N-2,1,1) - E(N-1,1,0) - E(N-1,0,1) + E(N,0,0) + B\Delta V, \quad (10)$$

$$\Delta V = (V(N-2,1,1) - V(N-1,1,0) - V(N-1,0,1) + V(N,0,0))/(N-1), \quad (11)$$

where $E(N,x,y)$ donates the energy of the system with N Ni atoms, x solute atoms and y vacancies occupying $N+x+y$ lattice sites; $V(N,x,y)$ represents the volume of the system with N Ni atoms, x solute atoms and y vacancies occupying $N+x+y$ lattice sites.

So the vacancy formation energy for an atom adjacent to a solute is

$$E_{\rm f}^{\rm v} = E_{\rm f}^{\rm s-v} + E_{\rm f}^{\rm V(Ni)}. \quad (12)$$

The diffusion barrier of the atom (E_i) is

$$E_i = E_{i-\rm saddle} - E_{i-\rm stable} + B(V_{i-\rm saddle} - V_{i-\rm stable}). \quad (13)$$

Here, $E_{i-\rm saddle}$ and $E_{i-\rm stable}$ are the energies of solute at the saddle point and the initial stable point,

respectively. $V_{i-\mathrm{saddle}}$ and $V_{i-\mathrm{stable}}$ are the volumes of solute at the saddle point and initial stable point, respectively. The activation energy (Q_a) for a solute is calculated by

$$Q_\mathrm{a} = E_\mathrm{f}^\mathrm{v} + E_2. \tag{14}$$

3. Results and discussion

The calculated vacancy formation energy $E_\mathrm{f}^{\mathrm{V(Ni)}}$ and diffusion barrier energy (E_b) for Ni self-diffusion are 1.677 eV and 1.206 eV respectively. The Ni self-diffusion activation energy is 2.883 eV (278.2 kJ/mol), which fits very well with the experimental value of 285 kJ/mol.[30] Table 1 shows the values of atomic mass of the solute atom, atomic radius,[31] melting point,[32] vacancy formation energy adjacent to a solute (E_f^v), diffusion barrier energy (E_2), and activation energy (Q_a), E_1, E_3–E_4, and E_4 when $E_3 = E_0$. The values of activation energy Q_a are compared with the calculation results given by Krcmar *et al.*[10] and Janotti *et al.*[12] The calculated values of activation energy (Q_a) conform to the results in Refs. [10] and [12] very well except for the results for Cr, Ru, and Co. The values of vacancy formation energy (E_f^v) for different solutes vary within 0.2 eV, and both the values of migration energy (E_2) and the values of activation energy (Q_a) are sorted in the following order: Al<Ta<Cr<Mo<Co<Ni<Ru<W<Re. So the major contribution to the activation energy (Q_a) comes from the solute diffusion barrier energy (E_2).

Table 1. Values of atomic mass of the solute atom, atomic radius,[31] melting point,[32] calculated vacancy formation energy adjacent to a solute (E_f^v), diffusion barrier energy (E_2), and the activation energy (Q_a), E_1, E_3–E_4, and E_4 when $E_3 = E_0$. All the energies are in units eV.

Element	m	r/Å	T_m/K	E_f^v	E_2	Q_a	Q_a[10,12]	E_1	E_3–E_4	E_4 ($E_3 = E_0$)
Ni	58.69	1.24	1726.15	1.677	1.206(E_0)	2.883	2.86			
Al	26.98	1.43	933.52	1.564	0.661	2.225		1.175	–0.068	1.274
Mo	95.94	1.39	2890.15	1.664	1.099	2.763	2.75	1.240	–0.247	1.453
Co	58.93	1.25	1768.15	1.710	1.164	2.874	3.00	0.734	–0.084	1.290
Ta	180.95	1.46	3269.15	1.545	0.758	2.304	2.35	1.378	–0.195	1.401
Ru	101.07	1.34	2523.15	1.649	1.263	2.912	3.15	1.009	–0.100	1.306
W	183.84	1.39	3683.15	1.694	1.289	2.983	3.05	1.234	–0.170	1.376
Cr	52.00	1.28	2130.15	1.721	0.942	2.663	3.04	0.963	–0.213	1.419
Re	186.21	1.37	3453.15	1.747	1.576	3.324	3.49	1.184	–0.244	1.450

Since $w_{3\mathrm{c}}$ is the host atom jump that dissociates the solute-vacancy pair, and it is the fourth nearest neighbouring position that is most similar to the bulk position, we assume that $E_3 = E_0$ in calculating E_4, which is reasonable. For example, all the calculated values of E_3 are within 0.03 eV off those of the solvent (Cu, Ag, Au, Ni, Pd, Pt) self-diffusion (E_0) in Adams *et al.*'s work,[16] and Janotti *et al.*[12] found that the E_3 is independent of solute atom size and nearly identical to that of solvent self-diffusion. There is E_3–$E_4 < 0$ for all the solutes, which means that the energy that Ni jumps needs for dissociating the solute–vacancy pair is lower than the energy needed for "associating" the solute–vacancy pair. Since E_3–$E_4 < 0$, and it can be inferred that $w_4/w_3 > 1$ from Eq. (8), $F(w_4/w_0) < F(1) = 0.7356$. The jump energies for Ni to induce the rotation of the solute–vacancy pair (E_1) are sorted in the following order: Co<Cr<Ru<Al<Re<W<Mo<Ta. In Janotti *et al.*'s work,[12] they found that as solute size increases, the E_1 also increases, since the diffusion of the solvent atom is subjected to a greater stress from the large solute atoms than that from small atoms at the saddle position. The atomic radii for transition elements are sorted in the following order: Co<Cr<Ru<Re<Mo≈W<Ta, showing that there are positive correlations between the atomic radius and E_1 value for transition elements. The Al element is an exception, one possible reason could be that Al is not a transition element, while the other elements are transition elements.

Figure 2 shows the values of f_2 for different solutes in Ni at various temperatures. The diffusion correlation factors of Re, Co, W, and Ru decrease with temperature increasing since $E_2 > E_1$, while the diffusion correlation factors of Cr, Mo, Ta, and Al increase with temperature increasing since their $E_2 < E_1$. The values of E_2–E_1 of transition elements are sorted in the

following order: Co>Re>Ru>W>Cr>Mo>Ta. At temperatures below 700 K, the values of f_2 are sorted in this order too, which shows that there are positive correlations between the values of E_2–E_1 and f_2 at low temperatures.

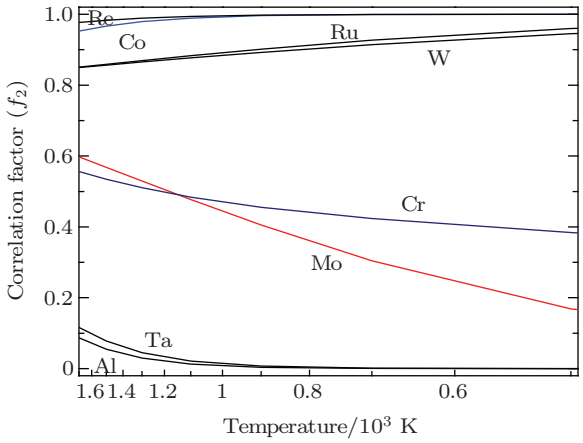


Fig. 2. (colour online) Variations of correlation factor (f_2) of different solutes with temperature.

Figure 3 illustrates the corresponding values of D_2/D_0 at different temperatures. The calculated diffusion coefficients are sorted in the following order: $D_{\rm Al} > D_{\rm Cr} > D_{\rm Co} > D_{\rm Ta} > D_{\rm Mo} > D_{\rm Ru} > D_{\rm W} > D_{\rm Re}$, which are consistent with the experimental results. The calculated solute diffusion coefficients and some corresponding experimental data from Refs. [33]–[40] (Al,[33] Mo,[34,35] Co,[36] Ta,[37] Ru,[38,39] W,[37] Cr,[33] Re[37,39,40]) are shown in Figs. 4(a)–4(h). The experimental interdiffusion coefficients are estimated by analysing the measured diffusion profiles from diffusion couples. The calculation results are in excellent agreement with the experimental data except that there are some discrepancies in the diffusion coefficient of Mo.

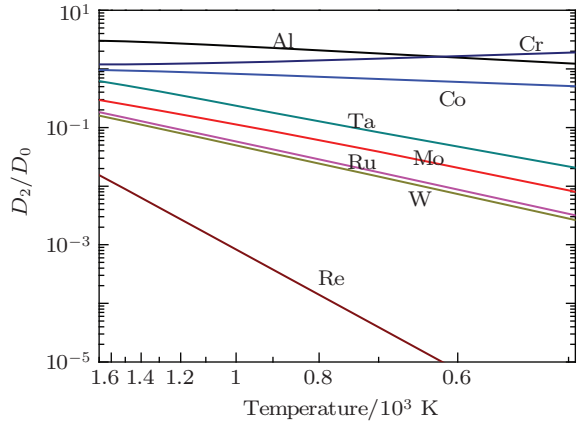


Fig. 3. (colour online) Calculated values of D_2/D_0 at different temperatures.

As the value of f_2 calculated from formula (3) slightly deviates from the Arrhenius change, the calculated diffusion coefficient as a function of temperature does not accurately follow the Arrhenius law in the form of $D = D_0 \exp(-Q/T)$. However, it is very close to one. We determine an effective total diffusion activation energy (Q) and pre-exponential factor (D_0) by fitting the obtained diffusion coefficients shown in Figs. 4(a)–4(h). The obtained Q and D_0 are listed in Table 2 and compared with experimental data.[3,33,38] The obtained values of Q are in excellent agreement with the experimental results except that there are some deviations for Mo, Ta, and Re. Note that the fitted Q is different from the $Q_{\rm a}$. In the value of $Q_{\rm a}$ the jumps of the surrounding solute atom that may affect the diffusion energy are neglected, while for the value of Q the contributions of the surrounding solute atoms are included. The obtained values of Q are larger than those of $Q_{\rm a}$. The surrounding Ni atoms contribute to the diffusion rates of the solutes considerably.

The D_0 determines the theoretical ultimate diffusion coefficient at the infinite temperature, while Q determines the changing extent as the temperature changes. If $Q < Q_{\rm Ni}$, then the D_2/D_0 value will decrease as the temperature increases, for example, in the case of Cr. If $Q > Q_{\rm Ni}$, then the D_2/D_0 value will increase as the temperature increases like in the cases of Al, Co, Ta, Ru, Mo, W, and Re. It can be seen that the trend in the diffusion coefficient is influenced by both the activation energy (Q) and diffusion pre-exponential factor D_0. For instance, although Cr has a lower value of Q than Al, the value of D_0 of Cr is lower than that of Al. The diffusion rates of Cr are slower than those of Al at temperatures above 700 K. According to the ubiquitous Meyer–Neldel compensation law,[41] the solute atom with a large activation energy also has a large diffusion pre-exponential factor. The obtained results conform to this law.

Janotti *et al.*[12] presented that the larger atoms have a lower diffusion barrier and diffusion activation energy for atoms in the same series. For Ta, W and Re in the 5d TM (transition metal) series, their atomic radii are sorted in the following order: Ta>W>Re and their values of Q are in the order, Ta<W<Re. The values of D are in the order, Ta>W>Re. For Mo and Ru in the 4d series, $r_{\rm Mo} > r_{\rm Ru}$, $Q_{\rm a}$ (Mo<Ru), Q (Mo<Ru), D (Mo>Ru). For Cr and Co in 3d series, r (Cr>Co), Q (Cr<Co), $Q_{\rm a}$ (Cr<Co), D (Cr>Co). So the larger atoms in the same series have lower diffusion barrier energies and faster diffusion rates, which conforms to the Janotti results.[12]

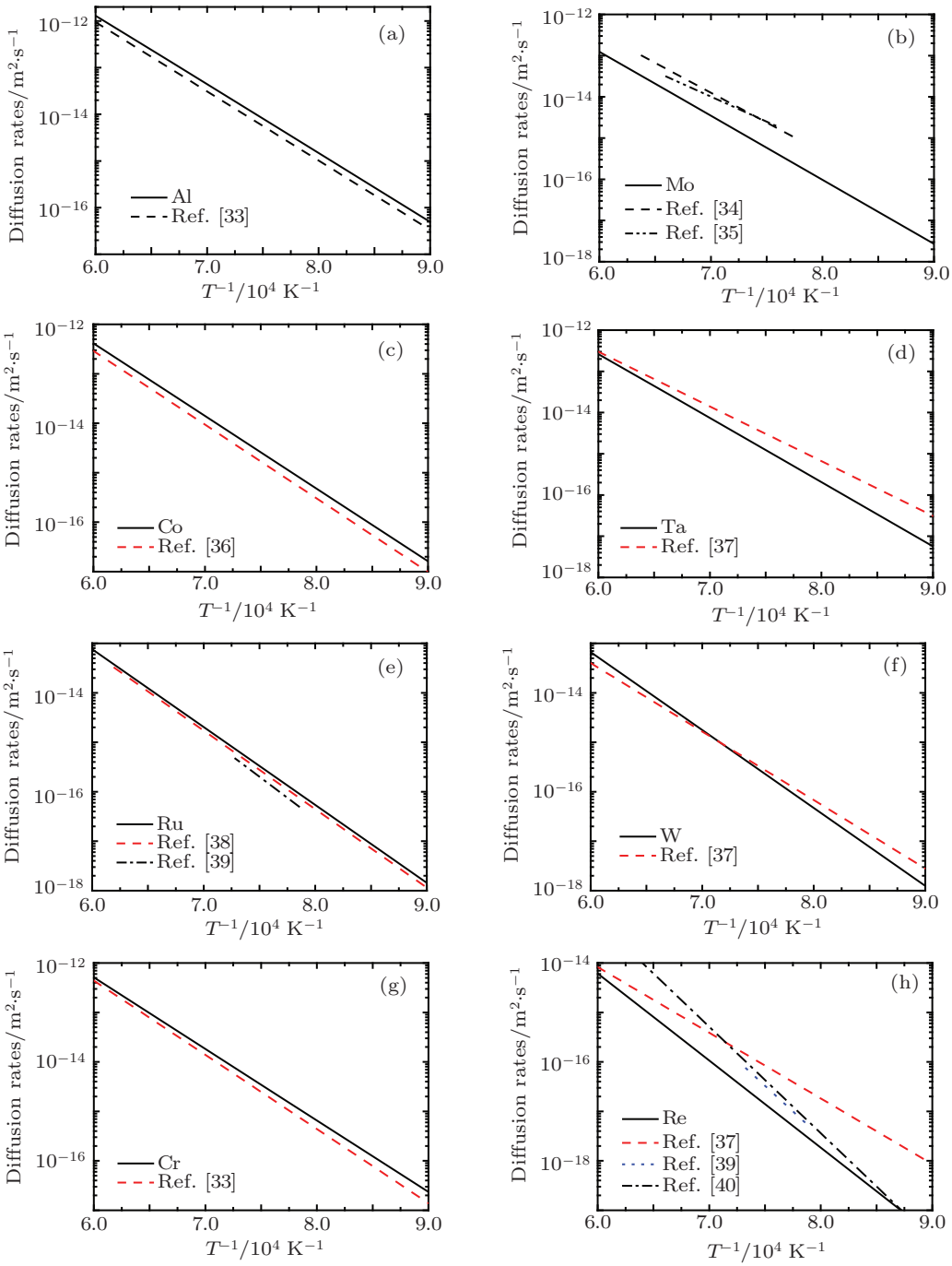


Fig. 4. (colour online) Calculated diffusion coefficients of different solutes ((a) Al, (b) Mo, (c) Co, (d) Ta, (e) Ru, (f) W, (g) Cr, (h) Re in FCC Ni), and their comparisons with experimental data.

Table 2. Calculated values of diffusion activation energy Q and pre-exponential factor (D_0) by fitting the obtained diffusion coefficients shown in Figs. 4(a)–4(h) and the corresponding cited values.

Elements	Al	Mo	Co	Ta	Ru	W	Cr	Re
D_0/m^2·s^{-1}	9.03×10^{-4}	4.32×10^{-4}	2.97×10^{-4}	5.13×10^{-4}	2.38×10^{-4}	2.10×10^{-4}	2.00×10^{-4}	2.35×10^{-4}
Q/eV	2.93	3.13	2.92	3.08	3.13	3.14	2.85	3.50
Q/kJ	282.68	301.68	282.18	297.19	302.28	302.51	274.91	337.50
D_0/m^2·s^{-1}[38]					2.48×10^{-4}			
Q/kJ[38]					304.40			
D_0/m^2·s^{-1}[33]	7.52×10^{-4}	7.04×10^{-5}	2.94×10^{-4}	6.71×10^{-5}		2.79×10^{-5}	4.33×10^{-4}	3.28×10^{-6}
Q/kJ[33]	284.00	267.59	284.17	267.73		282.13	287.00	278.82
D_0/m^2·s^{-1}[3]				1.98×10^{-6}		3.90×10^{-4}		2.18×10^{-7}
Q/kJ[3]				226.30		312.16		245.03

For the 8 elements calculated in this study, the diffusion coefficients correlate with their atomic numbers except for Ta, that is, the lighter the solute atom, the greater its diffusion coefficient in Ni is. For example, the atomic number increases in the order Al, Cr, Co, Mo, Ru, W, Re, and the diffusion coefficients decrease in this order, too.

4. Conclusions

The diffusion process in a Ni-based superalloy is important for comprehensively evaluating the regularity of influencing properties of the superalloys. A theoretical approach is used to predict the diffusion coefficients of alloying elements (Al, Mo, Co, Ta, Ru, W, Cr, Re) in Ni. The correlation factors from the 5-frequency model for impurity diffusion in an FCC lattice are computed with the first-principles DFT methods. Al is predicted to be the fastest diffusion impurity in Ni, and Re is the slowest diffusion impurity in the eight impurities under study. The diffusion coefficients are sorted in the following order: $D_{\mathrm{Al}} > D_{\mathrm{Cr}} > D_{\mathrm{Co}} > D_{\mathrm{Ta}} > D_{\mathrm{Mo}} > D_{\mathrm{Ru}} > D_{\mathrm{W}} > D_{\mathrm{Re}}$ above 700 K. The calculated diffusion coefficients are in good agreement with the experimental results. The total diffusion activation energy (Q) and pre-exponential factor (D_0) are obtained by fitting the obtained diffusion coefficients. It is found that there is a positive correlation between the atomic size of the solute and the E_1 value (the jump energy of the Ni atom that results in the rotation of the solute–vacancy pair). The value of E_2–E_1 (E_2 is the solute diffusion energy) and the correlation factor also show a positive correlation. A large atom in the same series has a low diffusion activation energy and a large diffusion coefficient.

Acknowledgment

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