Data Article

Data set for diffusion coefficients and relative creep rate ratios of 26 dilute Ni-X alloy systems from first-principles calculations

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A comprehensive first-principles study of solute elements in dilute Ni alloys: Diffusion coefficients and their implications to tailor creep rate by Hargather et al. [1].

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1. Computational methodology

Dilute solute diffusion coefficients as a function of temperature were calculated in the present work using density functional theory within the confines of the 5-frequency model [2,3]. 26 solute atoms were studied in the present work: Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Os, Pd, Pt, Re, Rh, Ru, Sc, Si, Ta, Tc, Ti, V, W, Y, Zn, and Zr.

Total energy calculations are carried out for a 32-atom supercell using the plane wave density functional code, Vienna ab-initio Simulation Package (VASP) [4]. A constant plane wave energy cutoff of 350 eV is used for all calculations, which is 1.3 times the default plane wave energy cutoff of nickel and larger than plane wave energy cutoff of all other solute atoms considered. A Monkhorst-Pack k-mesh scheme is used for all calculations, with a sampling of 8 × 8 × 8 for each system studied. For relaxation during the VASP calculations, the Methfessel-Paxton smearing method [5] is used for the calculation of forces acting on the atoms, and a final static calculation is performed after each relaxation using the linear tetrahedron method with Blöchl’s [6] correction for an accurate total energy calculation. Total electronic energy is converged to be at least 10⁻⁵ eV/atom. Due to the ferromagnetism of nickel up until its Curie point, [7], all calculations are performed in the present work within the spin polarized approximation. Further details of diffusion and computational theory can be found in the main article by Hargather et al. [1].

2. Data

2.1. 0 K results

Fig. 1 shows the effect of having one solute atom and no vacancies present in the 32-atom Ni supercell at 0 K on the following properties: equilibrium volume \( V_0 \), bulk modulus, \( B_0 \), first derivative
2.2. Atomic jump frequencies and thermodynamic parameters for all 26 Ni\textsubscript{31}X systems

The data in this section presents all factors relating to dilute solute diffusion as a function of temperature for all 26 Ni\textsubscript{31}X systems studied in the present work. Data is presented at \( T = 700 \) K and \( T = 1700 \) K. A detailed explanation of each of the jump frequencies and importance of the thermodynamic parameters can be found in the main article by Hargather et al. [1]. Table 1 gives the Gibbs energy of migration for each jump in the 5-frequency model for each of the 26 solutes in a Ni host lattice at the designated temperatures.

Table 2 presents all of the thermodynamic factors entering into dilute solute diffusion for all 26 Ni\textsubscript{31}X systems studied in the present work. The thermodynamic factors include the correlation factor, \( f_2 \), the enthalpy of vacancy formation adjacent to the solute, \( \Delta H_f \), the enthalpy of migration of the solute atom moving into an adjacent vacancy, \( \Delta H_m \), the entropy of vacancy formation adjacent to a solute, \( \Delta S_f \), entropy of migration of the solute atom, \( \Delta S_m \), and the temperature dependence of the correlation factor, \( C \).
Table 1
Gibbs energy of migration, $\Delta G_m$, for each of the five jump frequencies for dilute solute diffusion of all 26 Ni$_3$X systems studied in the present work.

| Solute | Temp, (K) | $\Delta G_{m0}$ (eV) | $\Delta G_{m1}$ (eV) | $\Delta G_{m2}$ (eV) | $\Delta G_{m3}$ (eV) | $\Delta G_{m4}$ (eV) |
|--------|-----------|----------------------|----------------------|----------------------|----------------------|----------------------|
| Al     | T = 700 K | 1.12                 | 1.36                 | 0.79                 | 1.29                 | 1.11                 |
|        | T = 1700 K| 1.07                 | 1.43                 | 0.86                 | 1.34                 | 1.19                 |
| Co     | T = 700 K | 1.12                 | 1.24                 | 1.38                 | 1.23                 | 1.27                 |
|        | T = 1700 K| 1.07                 | 1.27                 | 1.41                 | 1.27                 | 1.32                 |
| Cr     | T = 700 K | 1.12                 | 1.18                 | 1.30                 | 1.20                 | 1.27                 |
|        | T = 1700 K| 1.07                 | 1.25                 | 1.20                 | 1.19                 | 1.32                 |
| Cu     | T = 700 K | 1.12                 | 1.27                 | 0.98                 | 1.25                 | 1.17                 |
|        | T = 1700 K| 1.07                 | 1.34                 | 1.04                 | 1.31                 | 1.24                 |
| Fe     | T = 700 K | 1.12                 | 1.29                 | 1.20                 | 1.23                 | 1.25                 |
|        | T = 1700 K| 1.07                 | 1.33                 | 1.26                 | 1.27                 | 1.32                 |
| Hf     | T = 700 K | 1.12                 | 1.73                 | 0.40                 | 1.36                 | 0.79                 |
|        | T = 1700 K| 1.07                 | 1.75                 | 0.51                 | 1.40                 | 0.92                 |
| Ir     | T = 700 K | 1.12                 | 1.41                 | 1.72                 | 1.07                 | 1.17                 |
|        | T = 1700 K| 1.07                 | 1.46                 | 1.77                 | 1.14                 | 1.25                 |
| Mn     | T = 700 K | 1.12                 | 1.24                 | 0.95                 | 1.35                 | 1.27                 |
|        | T = 1700 K| 1.07                 | 2.02                 | 1.72                 | 2.23                 | 1.45                 |
| Mo     | T = 700 K | 1.12                 | 1.44                 | 1.31                 | 1.15                 | 1.07                 |
|        | T = 1700 K| 1.07                 | 1.48                 | 1.37                 | 1.20                 | 1.18                 |
| Nb     | T = 700 K | 1.12                 | 1.58                 | 0.76                 | 1.24                 | 0.92                 |
|        | T = 1700 K| 1.07                 | 1.60                 | 0.85                 | 1.27                 | 1.03                 |
| Os     | T = 700 K | 1.12                 | 1.38                 | 1.89                 | 1.06                 | 1.21                 |
|        | T = 1700 K| 1.07                 | 1.42                 | 1.95                 | 1.14                 | 1.32                 |
| Pd     | T = 700 K | 1.12                 | 1.44                 | 1.11                 | 1.19                 | 1.04                 |
|        | T = 1700 K| 1.07                 | 1.49                 | 1.18                 | 1.25                 | 1.13                 |
| Pt     | T = 700 K | 1.12                 | 1.43                 | 1.37                 | 1.13                 | 1.07                 |
|        | T = 1700 K| 1.07                 | 1.47                 | 1.42                 | 1.18                 | 1.15                 |
| Re     | T = 700 K | 1.12                 | 1.38                 | 1.89                 | 1.09                 | 1.18                 |
|        | T = 1700 K| 1.07                 | 1.44                 | 1.97                 | 1.16                 | 1.31                 |
| Rh     | T = 700 K | 1.12                 | 1.41                 | 1.40                 | 1.13                 | 1.14                 |
|        | T = 1700 K| 1.07                 | 1.44                 | 1.43                 | 1.18                 | 1.21                 |
| Ru     | T = 700 K | 1.12                 | 1.39                 | 1.51                 | 1.09                 | 1.16                 |
|        | T = 1700 K| 1.07                 | 1.42                 | 1.53                 | 1.15                 | 1.24                 |
Table 1 (continued)

| Solute | Temp, (K) | $\Delta G_{m0}$ (eV) | $\Delta G_{m1}$ (eV) | $\Delta G_{m2}$ (eV) | $\Delta G_{m3}$ (eV) | $\Delta G_{m4}$ (eV) |
|--------|-----------|----------------------|----------------------|----------------------|----------------------|----------------------|
| Sc     | T = 700 K | 1.12                 | −0.65                | 0.81                 | 1.12                 | 0.78                 |
|        | T = 1700 K| 1.07                 | 0.15                 | 1.65                 | 1.89                 | 1.93                 |
| Si     | T = 700 K | 1.12                 | 1.12                 | 0.95                 | 1.34                 | 1.22                 |
|        | T = 1700 K| 1.07                 | 1.16                 | 0.99                 | 1.28                 | 1.37                 |
| Ta     | T = 700 K | 1.12                 | 1.56                 | 0.92                 | 1.21                 | 0.95                 |
|        | T = 1700 K| 1.07                 | 1.59                 | 1.02                 | 1.24                 | 1.06                 |
| Tc     | T = 700 K | 1.12                 | 1.38                 | 1.57                 | 1.10                 | 1.16                 |
|        | T = 1700 K| 1.07                 | 1.42                 | 1.63                 | 1.15                 | 1.25                 |
| Ti     | T = 700 K | 1.12                 | 1.43                 | 0.61                 | 1.28                 | 1.02                 |
|        | T = 1700 K| 1.07                 | 1.46                 | 0.69                 | 1.31                 | 1.11                 |
| V      | T = 700 K | 1.12                 | 1.26                 | 1.09                 | 1.22                 | 1.17                 |
|        | T = 1700 K| 1.07                 | 1.29                 | 1.15                 | 1.24                 | 1.25                 |
| W      | T = 700 K | 1.12                 | 1.45                 | 1.50                 | 1.13                 | 1.09                 |
|        | T = 1700 K| 1.07                 | 1.51                 | 1.60                 | 1.20                 | 1.22                 |
| Y      | T = 700 K | 1.12                 | 2.42                 | 0.25                 | 0.26                 | −1.28                |
|        | T = 1700 K| 1.07                 | 2.45                 | 0.40                 | 0.41                 | −0.79                |
| Zn     | T = 700 K | 1.12                 | 1.34                 | 0.80                 | 1.31                 | 1.11                 |
|        | T = 1700 K| 1.07                 | 1.41                 | 0.89                 | 1.38                 | 1.18                 |
| Zr     | T = 700 K | 1.12                 | 1.82                 | 0.27                 | 0.14                 | −0.66                |
|        | T = 1700 K| 1.07                 | 1.80                 | 0.35                 | 0.20                 | −0.60                |

Table 2

Thermodynamic parameters at 700 K and 1700 K given for all factors entering into vacancy mediated dilute solute diffusion for the 26 Ni$_3$X systems studied in the present work. Calculated values include the correlation factor, $f_2$, the enthalpy of vacancy formation adjacent to the solute, $\Delta H_f$, the enthalpy of migration of the solute atom moving into an adjacent vacancy, $\Delta H_m$, the entropy of vacancy formation adjacent to a solute, $\Delta S_f$, entropy of migration of the solute atom, $\Delta S_m$, and the temperature dependence of $f_2$, $C$.

| Solute | Temp, (K) | $f_2$ | $\Delta H_f$ (eV) | $\Delta H_m$ (eV) | $\Delta S_f$ (kB) | $\Delta S_m$ (kB) | C (eV) |
|--------|-----------|-------|-------------------|-------------------|-------------------|-------------------|--------|
| Al     | T = 700 K | 0.0006| 1.62              | 0.75              | 2.13              | −0.607            | 0.532  |
|        | T = 1700 K| 0.104 | 1.69              | 0.70              | 2.84              | −1.11             | 0.482  |
| Co     | T = 700 K | 0.973 | 1.70              | 1.37              | 1.95              | −0.17             | −0.004 |
|        | T = 1700 K| 0.896 | 1.76              | 1.33              | 2.55              | −0.60             | −0.016 |
| Cr     | T = 700 K | 0.951 | 1.71              | 1.36              | 1.72              | 0.97              | −0.009 |
|        | T = 1700 K| 0.755 | 1.76              | 1.41              | 2.20              | 1.41              | −0.056 |
| Cu     | T = 700 K | 0.030 | 1.62              | 0.96              | 2.17              | −0.38             | 0.273  |
|        | T = 1700 K| 0.340 | 1.69              | 0.88              | 2.92              | −1.12             | 0.181  |
### Table 2 (continued)

| Solute | Temp. (K) | \( f_2 \) | \( \Delta H_f \) (eV) | \( \Delta H_m \) (eV) | \( \Delta S_f \) (\( k_B \)) | \( \Delta S_m \) (\( k_B \)) | C (eV) |
|--------|-----------|------------|-----------------|-----------------|----------------|----------------|--------|
| Fe     | T = 700   | 0.614      | 1.71            | 1.18            | 1.97          | −0.35          | 0.020  |
|        | T = 1700  | 0.725      | 1.79            | 1.12            | 2.69          | −0.91          | 0.014  |
| Hf     | T = 700   | 0.000      | 1.35            | 0.34            | 1.80          | −0.98          | 1.022  |
|        | T = 1700  | 0.005      | 1.43            | 0.27            | 2.54          | −1.60          | 1.172  |
| Ir     | T = 700   | 1.000      | 1.66            | 1.69            | 1.90          | −0.38          | 0.000  |
|        | T = 1700  | 0.995      | 1.72            | 1.64            | 2.50          | −0.93          | −0.003 |
| Mn     | T = 700   | 0.010      | 1.87            | 0.60            | 7.35          | −5.87          | 0.345  |
|        | T = 1700  | 0.159      | 3.02            | −0.10           | 18.21         | −12.44         | 0.125  |
| Mo     | T = 700   | 0.970      | 1.65            | 1.27            | 1.75          | −0.52          | −0.004 |
|        | T = 1700  | 0.898      | 1.70            | 1.22            | 2.19          | −1.04          | −0.015 |
| Nb     | T = 700   | 0.000      | 1.52            | 0.71            | 1.80          | −0.76          | 0.554  |
|        | T = 1700  | 0.123      | 1.58            | 0.66            | 2.40          | −1.28          | 0.495  |
| Os     | T = 700   | 1.000      | 1.70            | 1.87            | 1.80          | −0.44          | 0.000  |
|        | T = 1700  | 0.998      | 1.77            | 1.81            | 2.50          | −1.00          | −0.001 |
| Pd     | T = 700   | 0.366      | 1.57            | 1.09            | 2.17          | −0.41          | 0.079  |
|        | T = 1700  | 0.619      | 1.66            | 1.02            | 3.02          | −1.03          | 0.031  |
| Pt     | T = 700   | 0.993      | 1.58            | 1.36            | 2.06          | −0.26          | −0.002 |
|        | T = 1700  | 0.931      | 1.66            | 1.31            | 2.80          | −0.76          | −0.018 |
| Re     | T = 700   | 1.000      | 1.71            | 1.86            | 1.51          | −0.51          | 0.000  |
|        | T = 1700  | 0.998      | 1.76            | 1.79            | 1.95          | −1.21          | −0.001 |
| Rh     | T = 700   | 0.996      | 1.64            | 1.40            | 1.99          | −0.16          | −0.001 |
|        | T = 1700  | 0.935      | 1.68            | 1.37            | 2.39          | −0.43          | −0.020 |
| Ru     | T = 700   | 1.000      | 1.73            | 1.44            | 2.81          | −1.06          | 0.000  |
|        | T = 1700  | 0.973      | 1.98            | 1.25            | 4.17          | −1.96          | −0.013 |
| Sc     | T = 700 K | 1.0000     | 1.31            | 0.36            | 8.97          | −7.34          | 0.000  |
|        | T = 1700 K| 1.0000     | 1.85            | −0.18           | 14.09         | −12.51         | 0.000  |
| Si     | T = 700 K | 0.06       | 1.57            | 0.95            | 1.91          | −0.16          | 0.169  |
|        | T = 1700 K| 0.32       | 1.63            | 0.90            | 2.57          | −0.61          | 0.162  |
| Ta     | T = 700   | 0.010      | 1.58            | 0.86            | 1.72          | −0.91          | 0.383  |
|        | T = 1700  | 0.366      | 1.63            | 0.80            | 2.19          | −1.51          | 0.234  |
| Tc     | T = 700   | 1.000      | 1.69            | 1.55            | 1.80          | −0.35          | 0.000  |
|        | T = 1700  | 0.985      | 1.75            | 1.49            | 2.39          | −0.94          | −0.007 |
2.3. Dilute solute diffusivity plots

Additional plots of diffusivity as a function of 1000/T for the solute systems that were not presented in the main article [1] and have known experimental data are presented in this section. It should be noted that all of the plots are produced from data calculated directly from first-principles, and do not represent Arrhenius fits of data. The following plots in Figs. 2–15 are shown for 2nd row solute elements: Si, for 3d transition row solute elements: Ti, V, Cr, Mn, Fe, and Co, for 4d transition row solute elements: Zr and Mo, and for 5d transition row solute elements: Hf, Ta, W, Re, and Pt. The corresponding plots for the following solutes are shown in the main article [1]: Al, Cu, Nb, and W.

2.3.1. 2nd row solute elements

see Fig. 2.

![Fig. 2. Solute diffusion coefficient Si in Ni calculated in the present work (solid line) compared to poly-crystal data of Allison et al. [8] and Swalin et al. [9].](image_url)
2.3.2. 3d transition row solute elements

see Fig. 3.

![Graph Ti in Ni](image)

**Fig. 3.** Solute diffusion coefficient Ti in Ni calculated in the present work (solid line) compared to poly-crystal data of Bergner [10] and Swalin et al. [11].

![Graph V in Ni](image)

**Fig. 4.** Solute diffusion coefficient V in Ni calculated in the present work (solid line) compared to poly-crystal data of Murarka et al. [12].

![Graph Cr in Ni](image)

**Fig. 5.** Solute diffusion coefficient Cr in Ni calculated in the present work (solid line) compared to poly-crystal data of Monma et al. [13], Růžičková et al. [14], Tutunnik et al. [15], and Glinchuk et al. [16].
Fig. 6. Solute diffusion coefficient Mn in Ni calculated in the present work (solid line) compared to poly-crystal data of Swalin et al. [11].

Fig. 7. Solute diffusion coefficient Fe in Ni calculated in the present work (solid line) compared to single-crystal data of Bakker et al. [17], and to poly-crystal data of Guiardlenq [18] and Badia et al. [19].

Fig. 8. Solute diffusion coefficient Co in Ni calculated in the present work (solid line) compared to single-crystal data of Vladimirov et al. [20] and to poly-crystal data of Badia et al. [19], Hirano et al. [21], Hassner et al. [22], Divya et al. [23], and McCoy et al. [24].
2.3.3. 4d transition row solute elements

see Fig. 4.

![Graph showing solute diffusion coefficient Zr in Ni](image1)

**Fig. 9.** Solute diffusion coefficient Zr in Ni calculated in the present work (solid line) compared to poly-crystal data of Allison et al. [8] and Bergner [10].

![Graph showing solute diffusion coefficient Mo in Ni](image2)

**Fig. 10.** Solute diffusion coefficient Mo in Ni calculated in the present work (solid line) compared to poly-crystal data of Swalin et al. [9].

2.3.4. 5d transition row solute elements

see Fig. 5.

![Graph showing solute diffusion coefficient Hf in Ni](image3)

**Fig. 11.** Solute diffusion coefficient Hf in Ni calculated in the present work (solid line) compared to the poly-crystal data of Bergner [10].
Fig. 12. Solute diffusion coefficient Ta in Ni calculated in the present work (solid line) compared to the poly-crystal data of Bergner [10].

Fig. 13. Solute diffusion coefficient W in Ni calculated in the present work (solid line) compared to the single-crystal data of Vladimirov et al. [20], and the poly-crystal data of Bergner [10], Swalin et al. [11], and Monma [25].

Fig. 14. Solute diffusion coefficient Re in Ni calculated in the present work (solid line) compared to poly-crystalline diffusion couple experimental data by [26].
Table 3: Elastic [28] and stacking fault energy [29] data used for calculation of the relative creep rate ratio in the main article [1].

| Temp, (K) | Solute | $D$, m$^2$/sec | $b$, Å | $G$, GPa | $\gamma_{SFE}$, mJ/m$^2$ | $E$, GPa |
|----------|--------|----------------|--------|-----------|----------------|---------|
| 300 K    | Al     | 3.08E-54       | 1.447  | 86.31     | 109.15         | 223.38  |
|          | Co     | 1.14E-57       | 1.444  | 92.26     | 113.56         | 237.34  |
|          | Cr     | 3.50E-57       | 1.445  | 89.91     | 100.11         | 232.05  |
|          | Cu     | 1.88E-53       | 1.446  | 87.56     | 115.12         | 226.21  |
|          | Fe     | 3.07E-55       | 1.445  | 90.52     | 109.86         | 232.99  |
|          | Hf     | 1.39E-51       | 1.456  | 81.67     | 68.87          | 212.19  |
|          | Ir     | 1.58E-62       | 1.451  | 88.65     | 102.77         | 229.09  |
|          | Mn     | 1.77E-52       | 1.447  | 88.43     | 110.86         | 228.01  |
|          | Mo     | 1.95E-55       | 1.450  | 85.52     | 62.08          | 223.23  |
|          | Nb     | 2.77E-52       | 1.453  | 82.80     | 64.31          | 215.79  |
|          | Ni     | 2.31E-53       | 1.444  | 92.22     | 128.20         | 236.66  |
|          | Os     | 4.25E-66       | 1.450  | 91.74     | 86.31          | 236.58  |
|          | Pd     | 4.57E-52       | 1.451  | 87.98     | 118.12         | 226.82  |
|          | Pt     | 2.07E-55       | 1.452  | 88.96     | 121.06         | 229.68  |
|          | Re     | 1.90E-66       | 1.449  | 88.00     | 66.57          | 228.02  |
|          | Rh     | 5.49E-57       | 1.450  | 86.10     | 107.33         | 223.08  |
|          | Ru     | 2.53E-59       | 1.449  | 91.78     | 91.12          | 236.18  |
|          | Sc     | 2.88E-34       | 1.454  | 82.39     | 74.82          | 213.94  |
|          | Si     | 4.62E-51       | 1.444  | 85.79     | 112.50         | 222.85  |
|          | Ta     | 9.51E-53       | 1.453  | 83.10     | 71.44          | 216.82  |
|          | Tc     | 1.06E-60       | 1.449  | 89.72     | 71.08          | 231.67  |
|          | Ti     | 3.63E-54       | 1.449  | 86.42     | 83.08          | 223.79  |
|          | V      | 2.08E-54       | 1.446  | 87.41     | 81.33          | 226.56  |
|          | W      | 4.16E-59       | 1.450  | 85.93     | 66.54          | 223.45  |
|          | Y      | 3.32E-17       | 1.463  | 73.79     | 48.26          | 193.31  |
|          | Zn     | 4.81E-54       | 1.447  | 82.89     | 111.69         | 215.57  |
|          | Zr     | 3.85E-30       | 1.458  | 79.99     | 60.31          | 208.69  |

Fig. 15. Solute diffusion coefficient Pt in Ni calculated in the present work (solid line) compared to poly-crystalline diffusion couple experimental data by [27].
| Temp, (K) | Solute | \(D, \text{m}^2/\text{sec}\) | \(b, \text{Å}\) | \(G, \text{GPa}\) | \(\gamma_{\text{SFE}}, \text{mJ/m}^2\) | \(E, \text{GPa}\) |
|----------|--------|------------------|--------|--------|-------------------|--------|
| 600 K    | Al     | 1.38E-29         | 1.447  | 82.19  | 105.85            | 212.01 |
|          | Co     | 1.33E-31         | 1.444  | 87.82  | 109.79            | 225.37 |
|          | Cr     | 3.32E-31         | 1.445  | 84.98  | 99.05             | 218.59 |
|          | Cu     | 3.31E-29         | 1.446  | 83.60  | 111.26            | 215.20 |
|          | Fe     | 1.96E-30         | 1.445  | 86.80  | 106.45            | 222.45 |
|          | Hf     | 1.41E-28         | 1.456  | 78.26  | 66.57             | 202.18 |
|          | Ir     | 4.50E-34         | 1.451  | 83.34  | 99.59             | 214.86 |
|          | Mn     | 5.01E-29         | 1.447  | 84.36  | 107.40            | 216.68 |
|          | Mo     | 1.37E-30         | 1.450  | 80.99  | 60.20             | 211.41 |
|          | Nb     | 6.70E-29         | 1.453  | 79.30  | 62.37             | 205.87 |
|          | Ni     | 2.41E-29         | 1.444  | 87.91  | 124.22            | 224.72 |
|          | Os     | 6.77E-36         | 1.450  | 87.40  | 84.31             | 224.67 |
|          | Pd     | 1.07E-28         | 1.451  | 84.22  | 114.17            | 216.33 |
|          | Pt     | 1.84E-30         | 1.452  | 85.39  | 117.22            | 219.57 |
|          | Re     | 3.94E-36         | 1.449  | 83.80  | 64.89             | 216.37 |
|          | Rh     | 3.07E-31         | 1.450  | 83.93  | 103.97            | 216.39 |
|          | Ru     | 1.94E-32         | 1.449  | 87.03  | 88.40             | 223.30 |
|          | Sc     | 6.37E-20         | 1.454  | 78.82  | 71.85             | 204.08 |
|          | Si     | 2.62E-28         | 1.444  | 81.42  | 109.21            | 210.97 |
|          | Ta     | 3.99E-29         | 1.453  | 79.53  | 69.48             | 206.83 |
|          | Tc     | 3.57E-33         | 1.449  | 86.31  | 69.43             | 222.09 |
|          | Ti     | 1.21E-29         | 1.449  | 82.19  | 80.49             | 212.04 |
|          | V      | 7.98E-30         | 1.446  | 83.32  | 78.74             | 215.37 |
|          | W      | 1.71E-32         | 1.450  | 81.49  | 64.59             | 211.30 |
|          | Y      | 6.40E-12         | 1.463  | 70.09  | 45.49             | 183.50 |
|          | Zn     | 1.83E-29         | 1.447  | 79.26  | 107.92            | 205.41 |
|          | Zr     | 4.14E-18         | 1.458  | 76.41  | 58.12             | 198.75 |
| 900 K    | Al     | 2.67E-21         | 1.460  | 78.09  | 102.02            | 200.54 |
|          | Co     | 7.79E-23         | 1.458  | 83.25  | 105.42            | 212.92 |
|          | Cr     | 1.89E-22         | 1.460  | 80.55  | 97.81             | 206.30 |
|          | Cu     | 4.51E-21         | 1.459  | 79.40  | 106.78            | 203.60 |
|          | Fe     | 4.33E-22         | 1.459  | 82.79  | 102.51            | 211.77 |
|          | Hf     | 8.77E-21         | 1.469  | 74.45  | 63.95             | 191.98 |
|          | Ir     | 1.66E-24         | 1.464  | 78.43  | 95.93             | 201.56 |
|          | Mn     | 5.74E-21         | 1.460  | 79.93  | 103.39            | 204.32 |
|          | Mo     | 3.07E-22         | 1.463  | 76.52  | 58.03             | 199.39 |
|          | Nb     | 6.79E-21         | 1.467  | 75.43  | 60.16             | 194.99 |
|          | Ni     | 3.22E-21         | 1.458  | 83.41  | 119.62            | 212.43 |
|          | Os     | 9.62E-26         | 1.463  | 82.95  | 82.03             | 212.40 |
|          | Pd     | 7.51E-21         | 1.465  | 79.97  | 109.58            | 204.59 |
|          | Pt     | 4.64E-22         | 1.466  | 81.46  | 112.80            | 208.51 |
|          | Re     | 5.92E-26         | 1.462  | 79.64  | 62.96             | 204.68 |
|          | Rh     | 1.42E-22         | 1.463  | 81.32  | 100.08            | 208.54 |
|          | Ru     | 2.22E-23         | 1.463  | 81.84  | 85.28             | 209.27 |
|          | Sc     | 4.65E-15         | 1.468  | 74.85  | 68.41             | 193.15 |
|          | Si     | 1.26E-20         | 1.457  | 76.93  | 105.37            | 198.72 |
|          | Ta     | 4.89E-21         | 1.466  | 75.68  | 67.26             | 196.07 |
|          | Tc     | 6.45E-24         | 1.462  | 82.58  | 67.54             | 211.61 |
|          | Ti     | 2.79E-21         | 1.462  | 77.66  | 77.53             | 199.55 |
|          | V      | 1.24E-21         | 1.459  | 78.93  | 75.74             | 203.30 |
|          | W      | 1.49E-23         | 1.464  | 76.80  | 62.35             | 198.49 |
|          | Y      | 4.36E-10         | 1.478  | 66.07  | 42.28             | 172.76 |
|          | Zn     | 3.26E-21         | 1.461  | 75.37  | 103.55            | 194.51 |
|          | Zr     | 4.78E-14         | 1.471  | 72.51  | 55.63             | 187.98 |
2.4. Relative creep rate ratio data table

The diffusivity data from the present work is combined with the elastic constant calculations from Shang et al. [28] and the stacking fault energy calculations from Shang et al. [29] on the same 26 Ni31X systems to calculate a relative creep rate ratio. The relative creep rate ratio shows the effect of each solute element on the creep rate of the dilute Ni-X alloy compared to the creep rate of pure Ni. The data used for the relative creep rate ratio plots in the main article [1] is presented in Table 3.

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Transparency document. Supporting information

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Further reading

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