Erratum: First-principles characterization of Ni diffusion kinetics in $\beta$-NiAl


Kristen A. Marino and Emily A. Carter

(Received 25 July 2009; published 12 August 2009)


Equation (8) should read:

$$D = \left( \frac{1}{6} a^2 v_0 e^{(-\Delta S/k_B)} \right) e^{(-Q/k_BT)}.$$

There is an extra $T$ in the first exponential in the published paper.

The value of $\hbar$ was erroneously used instead of Planck’s constant, $h (h=2\pi \hbar)$, when calculating vibrational entropies using Eq. (9). The consequence of this error is that the values given for the entropic factors, $e^{(-\Delta S/k_B)}$, and diffusion constant pre-exponential factors, $D_0$, in Tables I, IIb, IIIb, IVb, and V are too large by a factor of $2\pi$. This error does not affect the overall trends or conclusions presented in the paper, but the agreement of the pre-exponential factors with experimental data is poorer than previously represented.