Erratum: Properties of liquid nickel: A critical comparison of EAM and MEAM calculations [Phys. Rev. B 65, 024209 (2002)]

F. J. Cherne, M. I. Baskes, and P. A. Deymier
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In Ref. 1 we presented a number of calculations for the viscosity and diffusivity predicted by a variety of potentials. In continuing our work we reevaluated some of the data and found that the potential we had called MEAM Ni3 in these calculations was not the Ni3 reported in Ref. 2. Therefore we here present the corrected calculations for MEAM Ni3. Figure 1 is the updated plot for Fig. 2 in the original paper. As a result of these changes the values for MEAM Ni3 in Table III should read 11.759 mPa s, 0.793 eV, and 4.86 ± 0.05 for η_0, E_a, and E_a/kT_m, respectively. Ni3's value in Table IV should read 7.41 mPa s for η_{calc}. All other values for Ni3 remain the same in Table IV. These modifications to MEAM Ni3 cause the points in Fig. 6 of the original paper to be beyond the range of the plot. Similarly Fig. 3 in the original paper should be as shown in Fig. 2 by using the appropriate potential in Ref. 2. Thus the values in Table V for Ni3 should be 60.14×10^{-5} cm^2/s for D_0, 0.511 for E_a, and 3.14 ± 0.04. By applying these changes our conclusions are slightly modified to state that the only MEAM potential that is in good agreement with experiment is MEAM Ni4. Thus we can conclude that the potential that has the best agreement with the coefficient of thermal expansion also has the best agreement with the liquid properties calculated in the original paper.

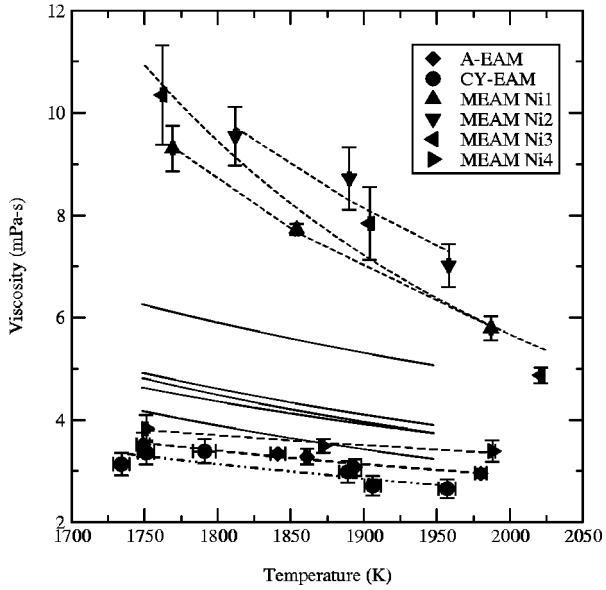

FIG. 1. Viscosity of liquid Ni as a function of temperature. See Ref. 1 for more details.

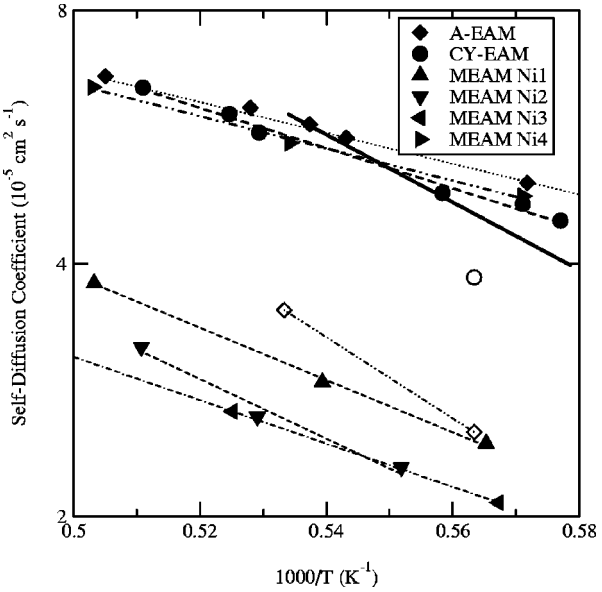

FIG. 2. Diffusivity of liquid Ni as a function of temperature. See Ref. 1 for more details.

[1] F.J. Cherne, M.I. Baskes, and P.A. Deymier, Phys. Rev. B **65**, 024209 (2002).
[2] M.I. Baskes, Mater. Chem. Phys. **50**, 152 (1997).

