Erratum: Composition, structure, and stability of $RuO_2(110)$ as a function of oxygen pressure [Phys. Rev. B 65, 035406 (2001)]

Karsten Reuter and Matthias Scheffler

(Received 14 January 2007; published 25 January 2007)

DOI: 10.1103/PhysRevB.75.049901 PACS number(s): 68.47.Gh, 05.70.Np, 71.15.Mb, 99.10.Cd

Our paper determines the lowest-energy structure of a $RuO_2(110)$ surface in thermodynamic equilibrium with an oxygen-rich environment. The limit of least oxygen-containing gas phase conditions considered (O-poor limit) is motivated by the Gibbs free energy of formation of the bulk oxide ΔG_f. Employing the value of $\Delta G_f(0,0)$ at 0 K, we stated the error as opposed to using the temperature and pressure dependent value $\Delta G_f(T,p)$ as 0.63 eV at 1000 K and 1 atm. This value was erroneously deduced from the CRC Handbook,[1] due to inconsistent entries in the $\Delta G_f(T,p^\circ=1\ \text{atm})$ table, mixing decadic and natural logarithms in the stated interpolation formulae for rutile structured oxides. Using the proper decadic logarithm in the interpolation formula for RuO_2 the correct variation up to 1000 K and 1 atm is 1.78 eV.[2] In addition, Eq. (19) in our paper contains an erroneous factor of 2 in the denominator, which leads to an estimate of the vibrational contribution to the surface free energy in Fig. 1 that is too small by a factor of 2. In the temperature range up to 600 K discussed in our paper, this contribution remains nevertheless below 10 meV/Å^2. Therefore neither error affects the conclusions drawn.

We thank Ian Grey for making us aware of the inconsistent entries in the CRC Handbook.

---

[1] *CRC Handbook of Chemistry and Physics*, 76th ed. (CRC Press, Boca Raton FL, 1995).
[2] H. St. C. O'Neill and J. Nell, Geochim. Cosmochim. Acta, Vol. **61**, 5279 (1997).

