Erratum: Diffusion of carbon in bcc Fe in the presence of Si [Phys. Rev. B 81, 054116 (2010)]

D. Simonovic, C. K. Ande, A. I. Duff, F. Syahputra, and M. H. F. Sluiter
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Table III and Fig. 7 should be replaced with those listed below.

Text on page 6 should read (starting with the last sentence of the first paragraph that ends on p. 6):

Just 2 at. % Si substitutionally dissolved in bcc Fe reduces the C diffusivity by 39% at 500 K and by 14% at 1000 K.

There are two mechanisms by which Si reduces the diffusivity of C: a) the first and second neighbor shells around Si are so high in energy that C is blocked from these sites, this reduces the number of positions through which C can diffuse (labyrinth mechanism); and b) at slightly greater distances C gets weakly trapped around Si so that it remains immobilized for some time, depending on the temperature (trapping mechanism[14]). The KMC simulations allow us to precisely pinpoint the contribution of each mechanism. When the attractive Si-C interactions in the third through sixth shells are set to zero, the C diffusion in Fe with 2 at. % Si is reduced by 10% both at 500 K and at 1000 K. This indicates that at 1000 K the labyrinth mechanism is the most important. When, instead simulations are repeated whereby the repulsive Si-C interactions in the first and second shells are set to zero, diffusivity in Fe with 2 at. % Si is reduced by 35% at 500 K and by 8% at 1000 K. This indicates that at 500 K the trapping mechanism is dominant, but that at 1000 K labyrinth and trapping mechanisms contribute about equally.

The last lines in the Sect. IV. SUMMARY should read:

The Si-C interaction is reflected also in the influence of Si on the C diffusivity: (I) at high temperatures of about 1000 K, the strong repulsion between C and Si in the first and second neighbor shells plays an important role. This causes a mild reduction in the C diffusivity because there are fewer diffusion paths as C is blocked from sites very close to Si. (II) at lower temperatures of about 500 K, the energetically weaker attraction plays a dominant role in reducing the diffusivity of C through entrapment of C at a large number of interstitial sites in the vicinity of Si. At 500 K, 1 at. % of Si in solution may reduce the diffusivity by as much as 22% relative to Si-free bcc Fe.

TABLE III. Simulated carbon diffusivity D (in m^2/s) in bcc Fe as function of silicon concentration C_{Si} at temperatures T of 500 K and 1000 K.

	T	
C_{Si}	500 K	1000 K
0	$5.92 \cdot 10^{-16}$	$9.00 \cdot 10^{-12}$
0.005	$5.20 \cdot 10^{-16}$	$8.61 \cdot 10^{-12}$
0.01	$4.62 \cdot 10^{-16}$	$8.38 \cdot 10^{-12}$
0.015	$4.11 \cdot 10^{-16}$	$8.04 \cdot 10^{-12}$
0.02	$3.63 \cdot 10^{-16}$	$7.74 \cdot 10^{-12}$

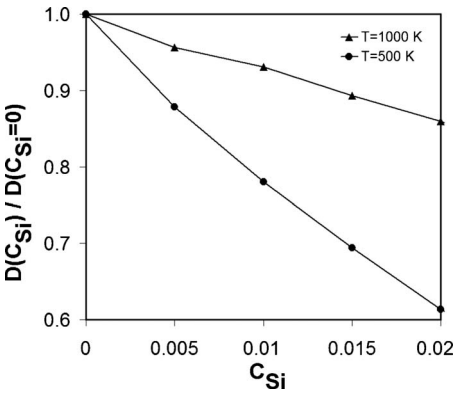

FIG. 7. Predicted C diffusion coefficient in the presence of substitutional Si relative to C diffusion coefficient in the absence of Si, in bcc Fe at temperatures of 500 K and 1000 K.

