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Carbon Interstitial Diffusion in γ-Fe

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Abstract

In this paper, we employ a four-frequency model for carbon diffusion in austenite where interstitials can diffuse either as isolated species or pairs. We make use of the Okamura and Allnatt formalism that has recently been shown to be near exact. The general finding of a previous analysis of McKee is confirmed: the increase of both tracer and chemical carbon diffusion coefficients with carbon composition at 1000°C is largely a result of a much higher rate of rotation of an interstitial pair compared with isolated interstitials. However, we find that the carbon atoms move almost two times faster as a rotating pair than found originally by McKee.

1. Introduction

Carbon diffusion in γ-Fe or austenite is a technologically important example of interstitial solute diffusion in a f.c.c. metal. The chemical diffusion coefficient has been measured at 802°C, 851°C and 1000°C, and as a function of carbon composition c [1]; the tracer carbon diffusion coefficient has been measured at 1000°C also as a function of composition [2]. These data have been analysed on many occasions with two different models [2-7]. The first is the lattice gas model in which effective nearest neighbour repulsive interactions are supposed between the interstitials [2-6]. In the second, appropriate for very low compositions, it is supposed that the diffusing species can diffuse *only* as isolated atoms or as bound pairs [7]. Four atom-vacant interstice frequencies are identified: the first, u_1, is a rotational frequency of one atom about the other when the interstitial atoms are paired, the second frequency, u_3, is the dissociative frequency of a nearest neighbour pair, the third frequency, u_4, is the associative exchange frequency to form a (nearest neighbour) pair, and the fourth frequency, u_0, is the frequency for jumps of isolated interstitials. Using the pair-association method, McKee [7] showed that the initial increase of both tracer and chemical diffusion coefficients with composition at 1000°C is largely a result of a high rate of rotation of an interstitial pair compared with isolated interstitials. Although a small effective repulsive interaction exists between interstitial atoms, once formed, a pair is the faster moving defect species. McKee assumed that after the dissociation of a bound pair the subsequent jumps are random in direction. Okamura and Allnatt (OA) avoided this assumption by employing linear response formulae. The calculated phenomenological coefficients were calculated exactly to first order in the concentrations of paired and unpaired species. Recent Monte Carlo calculations [9] show that OA's treatment [8] is essentially exact. However, the OA treatment has not been applied to carbon diffusion in austenite and is addressed here.

2. Theory

The differences between McKee's and OA's formalisms largely centre on the treatment of tracer correlation effects. Following McKee [7] we introduce the ratios of the exchange frequencies $x = u_1/u_3$, $y = u_4/u_3$ and $z = u_0/u_3$. Writing the enhancement of the tracer carbon diffusion coefficient as:

$$D^* \approx D(0)(1 + b_1^{(OA)tr} c)$$

we can show that the linear enhancement factor in the OA formalism [8] is given by:

$$b_1^{(OA)tr} = \frac{(14+4x)y}{z} - 12y + 7 - \frac{7(1-F)z(2u_1+7)}{y(2x+7F)}$$

$$+ \frac{56(1-F)z(x+1)}{2x+7F} - \frac{y(4x^2+6(5-7F)x+(16-7F))}{z(2x+7F)}$$

McKee's result is obtained simply by putting F=1.0 which corresponds to the assumption that after the dissociation of a bound pair the subsequent jumps are random in direction. On detailed comparison with the experimental diffusion data along with the carbon activity data (for the thermodynamic factor) we confirm the general finding of McKee [7] that the increase of both tracer and chemical carbon diffusion coefficients with composition at 1000°C in austenite is largely a result of a higher rate of rotation of an interstitial pair compared with isolated carbon atoms. The slight repulsive tendency between the carbon atoms prevents them from forming long-lived interstitial pairs. But once formed, a pair is the faster moving defect species. But the new analysis shows that the carbon atoms move much quicker as a rotating pair ($u_1/u_0 = x/z \approx 5.0$) compared with isolated atoms than was originally estimated by McKee ($x/z \approx 3.0$).

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