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Defect Calculations for Carbon Interstitials in α -Iron[†]

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A comparison is presented between real-space and reciprocal-space methods of performing lattice-defect calculations for carbon interstitials in α -iron. After correcting for several errors, no significant differences were found in the results of either method.

In an earlier defect calculation by Johnson, Dienes, and Damask¹ (JDD) for carbon interstitials in α -iron, an error was made in the published form of the potential-energy function derived for the carbon-iron interaction: Eq. (3) in JDD should read

$$\Phi(r) = 3.365(2.236 - r)^3 + 0.886r - 2.156.$$

The correct function was used in the calculations.

Flocken² has recently repeated these calculations using the carbon-iron and iron-iron interactions given by JDD but using a different method of calculation (JDD used a real-space "lattice plus elastic continuum" method while Flocken used a reciprocal-space "lattice-statics" method). Unfortunately, the incorrect potential from JDD was carried over to the Flocken calculation [Eq. (6) in Ref. 2]. However, in obtaining force equations from the carbon-iron potential an error in differentiation was made which, in effect, corrected the errant sign. Since the lattice-statics method is based on force equations, all ensuing computations for atomic displacements and relaxation energies are consistent with the correct carbon-iron potential. There is a typographical error in sign in Eq. (19) in Flocken, but the results are given with the correct sign. The relaxation energies calculated by JDD and Flocken are compared in Table I.

To determine the difference in energy between the octahedral and tetrahedral configurations, i. e., the carbon migration energy, the energy required to insert a carbon atom in the unrelaxed lattice must be added to the relaxation energy. Here the incorrect sign in the JDD calculation affects the

results reported by Flocken. The correct values are 0.420 eV for octahedral and 0.525 eV for tetrahedral configurations, which, when combined with the relaxation energies given in Table I, yield $E^m = 0.86$ eV for the JDD calculation and $E^m = 0.85$ eV for the Flocken calculation.

Since the strain field and the interaction energies between different pairs of carbon atoms reported in both calculations are in essential agreement, no significant differences exist between the results of the two calculations. Objections raised by Flocken to the use of an elastic continuum boundary condition in the real-space method are not sustained by the results. The constraint of requiring a harmonic approximation in the lattice-statics method appears to be more severe, since the relaxation energies are greater in magnitude in the real-space calculations, i. e., both methods seek to minimize configuration energy, and the real-space calculations arrive at a lower energy configuration.

Reference 2 is the sixth paper in a series by Flocken and Hardy³⁻⁷ using the lattice-statics method. The conclusion is consistently drawn that real-space calculations are inadequate and unreli-

TABLE I. Relaxation energies for carbon interstitials in α -iron.

Symmetry	Relaxation energy (eV)	
	JDD	Flocken
Octahedral	-1.742	-1.68
Tetrahedral	-0.987	-0.94

able for defect calculations. The lattice-statics method is often referred to as exact without an appropriate qualifier for the harmonic approximation. The present comparison (and indeed earlier comparisons) does not bear this out. This is admittedly a subjective judgement—Flocken and Hardy consider a 5–10% disagreement in displacements to be unsatisfactory, while the present author considers this to be a good agreement.

At the present time, it would seem that the most reliable method of calculation would be to use a

real-space lattice approach near the defect but to replace the elastic continuum component of the calculation with a lattice-statics calculations. The flexibility to investigate nonsymmetric configurations would be impaired by such a program, however, and the computer time to carry out such a calculation would be much greater than with other methods. The reliability of interatomic potentials is not sufficiently good at the present time to warrant such an approach except as an occasional check on more approximate methods.

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Pair Effects in Disordered Alloys*

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An error in keeping track of diagrams in the paper by Aiyer, Elliott, Krumhansl, and Leath is reported and corrected and a general rule for avoiding this kind of problem for larger clusters is presented. The recent work of Nickel and Krumhansl is shown to be in agreement with the corrected formula.

In a paper¹ (hereafter referred to as A) of a few years ago a general diagrammatic procedure for calculating configuration-averaged properties in disordered alloys was presented. In a recent paper Nickel and Krumhansl² have calculated the effects of the self-consistent scattering by pairs of defects in a generalization of the coherent-potential approximation which was in disagreement with the pair formula calculated in the last section of A. The purpose of this paper is to point out the omission in diagram counting that was made in that section, to show that, when corrected, there is full agreement with Ref. 2, and to emphasize that the diagrammatic technique presented in A, although at times tedious, is in fact correct and straightforward in its prescription for getting the proper generalization of the coherent-potential approximations.

We assume the reader's knowledge of the methods and notation of A and first point out the errors in Sec. VI of that paper. Then we show how this result could have been more simply obtained. Finally, we point out the equivalence of this work with that of Ref. 2.

The scattering by a pair of defects, which are a

distance \vec{R} apart, is calculated with the restriction $\vec{R} \neq 0$ strictly maintained so that there are no pair corrections to the single-site terms $\Sigma_s^1 = \tau'$ in Eq. (47) of A. [This statement is in contrast to the statement above Eq. (53).] We note that Eq. (47) can be written in the form

$$c\tau \langle G(0) \rangle = \tau' [G''(0)] / \{1 - \tau' [G''(0)] \langle G(0) \rangle\}, \quad (1)$$

where

$$G''(0) = \langle G(0) \rangle / \{1 - \tau' [\langle G''(0) \rangle] \langle G(0) \rangle\}.$$

The pair terms summed in A were just those diagrams shown below in the first column of Fig. 1 where the double horizontal line represents the full *off-diagonal* propagator $\langle G(\vec{R}) \rangle$, the wide solid horizontal line represents the full *diagonal* propagator $\langle G(\vec{0}) \rangle$, and the open-circle vertex represents the bare vertex, uncorrected for multiple occupancy. The higher columns contain the multiple-occupancy corrections (the solid circle represents the fully corrected vertex).

We now come to the basic omission in Sec. VI of A. In Eq. (58), which should have been the sum of all the columns of Fig. 1, the correction terms