A STUDY OF SMALL VACANCY CLUSTERS IN IRON USING MANY BODY POTENTIAL

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Abstract ·

Computer simulation techniques are employed to obtain binding energies of 2, 3 and 4 vacancy clusters in α –iron using the Finnis Sinclair many body potential. The results are compared with earlier pair potential calculations. The many body potential is found to be quite successful in simulating vacancy clusters.

Introduction

Macroscopic swelling due to void formation is a major issue in radiation damage. However, the physical mechanisms that comprise the void nucleation process are still not completely understood. A supersaturation of vacancies can be created in a metal by energetic particle irradiation, quenching or mechanical deformation. At the temperatures where the vacancy is mobile, these vacancies can migrate to form microscopic clusters. The final geometry of the resultant vacancy clusters can have a significant impact on the macroscopic behaviour of the metal. The formation of planar vacancy clusters such as dislocation loops tend to strengthen the metal. On the other hand, formation of three dimensional voids can produce a considerable amount of swelling. The clustering of vacancies in crystals to form dislocation loops and voids is an important phenomenon of the solid state. However, owing to the difficulties of making direct experimental observations on point defects and their interactions, the early stages of the clustering process are not well understood. Theoretical studies of the structures and energies of small vacancy clusters are thus needed.

The geometry of vacancy clusters in BCC crystals has been examined by various researchers [1-4]. Using pairwise potentials it is found that in BCC metals the second nearest neighbour di-vacancy is more stable than the first nearest

neighbour one. It was therefore necessary to extend the definition of close-packed clusters to include second nearest neighbours as well. This was done by Malik and Crocker [5] for all the BCC close-packed clusters with up to four vacancies. They also calculated the binding energies of these clusters using the Johnson J_0 pair potential [6].

In atomistic modeling of transition metals, pair potentials have been found to be insufficient to explain a number of observations. In any pure pairwise model, the Cauchy pressure $1/2 \ (C_{11}\text{-}C_{44})$ is necessarily zero and the free surface of a metal shows an outward relaxation, contrary to the experimental observations. With any pairwise potential, the vacancy formation energy is forced to be equal, apart from minor relaxation effects, to the energy of broken bonds, and therefore to the cohesive energy, where it is experimentally found to be one third of this value [7]. Besides these general drawbacks, the use of a pairwise potential has proven unsatisfactory in the study of certain properties of transition metals, such as the self-interstitial migration energy [8]. These inadequacies of the central potentials make their usefulness quite doubtful even for a qualitative analysis of many aspects of the defect physics of transition metals. The introduction of the Finnis Sinclair many body (FS) potential [9, 10] has been welcomed as a satisfactory alternative to the existing approaches [11-13]. It is necessary to investigate how successful these new potentials are in explaining the point defect structures in transition metals. The present work is an attempt to esti-

mate the capability of the FS potential when applied to small vacancy clusters in iron. The computational procedure and results are given in section 2 and their significance is discussed in section 3.

The Computational Procedure and Results

The model BCC crystals consisted of an inner computational cell of 1458 free atoms, in the form of a cube with 18 {100} planes, surrounded by an appropriate mantle of fixed atoms. The defect was introduced in the middle of the model. The model was allowed to relax to a minimum energy configuration using an iterative procedure.

The number of distinct configurations of close-packed clusters of 2, 3 and 4 vacancies at either first or second nearest neighbour sites in a BCC structure, are 2, 6 and 35, respectively. The structure of these clusters, projected onto the (110) plane, are shown in Figure 1. The binding energies of all the vacancy clusters have been evaluated using computer simulation methods and the FS potential for α-iron. The results obtained are given in Table 1 along with earlier calculations [5] using J_0 pair potential for comparison. The present results are somewhat higher than

the earlier values, because FS potential gives a higher vacancy formation energy of 1.81eV as compared to 1.37eV using J_0 potential. The FS potential is more satisfactory because the present value is closer to the experimental value of 1.79eV [7].

The new results confirm the earlier finding that the second nearest neighbour di-vacancy is more stable than the first nearest neighbour one. This effect is found to be reflected in all other binding energies obtained. For example, the straight <100> clusters (3.6, 4.35) have larger binding energies than the <111> linear clusters (3.3, 4.12). Also, the clusters with two or three B bonds (3.5, 4.30) have higher binding energies than comparable clusters with two or three A bonds (3.2, 4.8), where A, B, C, ---- refer to the 1st, 2nd, 3rd, ------- neighbour bonds. It is interesting to note that in clusters where AAACC bonds are involved (4.8, 4.9, 4.10) the binding energies are even lower than the corresponding pair potential values.

When interpreting the results, it must also be borne in mind that the range of J_0 potential excludes all bonds other than types A and B. Hence, the binding energies of the clusters are mostly determined by the number of A and B bonds, and to a first approximation the effects of C, D and

Table 1. Possible configuration of vacancy clusters in BCC metals. The columns give the configuration number (P.n), the bond classification (bonds), and the binding energies $E^b(J_0)$, E^b (FS) in electron-volts calculated using the J_0 pair potential and the FS many body potential for α-iron. The clusters are illustrated in Figure 1. The letters A, B, C,... are 1st, 2nd, 3rd,... neighbour distances.

| P. n	Bonds	$E^b(J_0)$	E^b(FS)	P.n	Bonds	$E^b(J_0)$	E^b(FS)
2.1	A	0.127	0.133	2.2	B	0.191	0.234
3.1	AAB	0.480	0.559	3.2	AAC	0.241	0.236
3.3	AAE	0.257	0.282	3.4	ABD	0.331	0.389
3.5	BBC	0.356	0.412	3.6	BBF	0.378	0.473
4.1	AAAABB	1.009	1.213	4.2	AAAABC	0.766	0.888
4.3	AAABBC	0.820	0.953	4.4	AAABBD	0.830	0.983
4.5	AAABCD	0.608	0.670	4.6	AAABCE	0.598	0.672
4.7	AAABDE	0.623	0.718	4.8	AAACCC	0.345	0.308
4.9	AAACCD	0.395	0.379	4.10	AAACCG	0.352	0.333
4.11	AAACEG	0.365	0.375	4.12	AAAEEJ	0.390	0.436
4.13	AABBCD	0.656	0.745	4.14	AABBDD	0.700	0.827
4.15	AABBDF	0.681	0.808	4.16	AABCDD	0.458	0.493
4.17	AABCDE	0.432	0.456	4.18	AABCDH	0.447	0.489
4.19	AABDDF	0.442	0.487	4.20	AABDDH	0.472	0.533
4.21	AABDDI	0.465	0.530	4.22	AABDEI	0.465	0.538
4.23	ABBCDD	0.510	0.570	4.24	ABBCDD	0.535	0.600
4.25	ABBCDG	0.492	0.557	4.26	ABBDDG	0.523	0.618
4.27	ABBDDK	0.532	0.635	4.28	ABBDFK	0.520	0.625
4.29	BBBBCC	0.737	0.867	4.30	BBBCCC	0.497	0.534
4.31	BBBCCE	0.518	0.578	4.32	BBBCCF	0.515	0.586
4.33	BBBCCH	0.515	0.590	4.34	BBBCFH	0.543	0.653
4.35	BBBFFO	0.561	0.716				
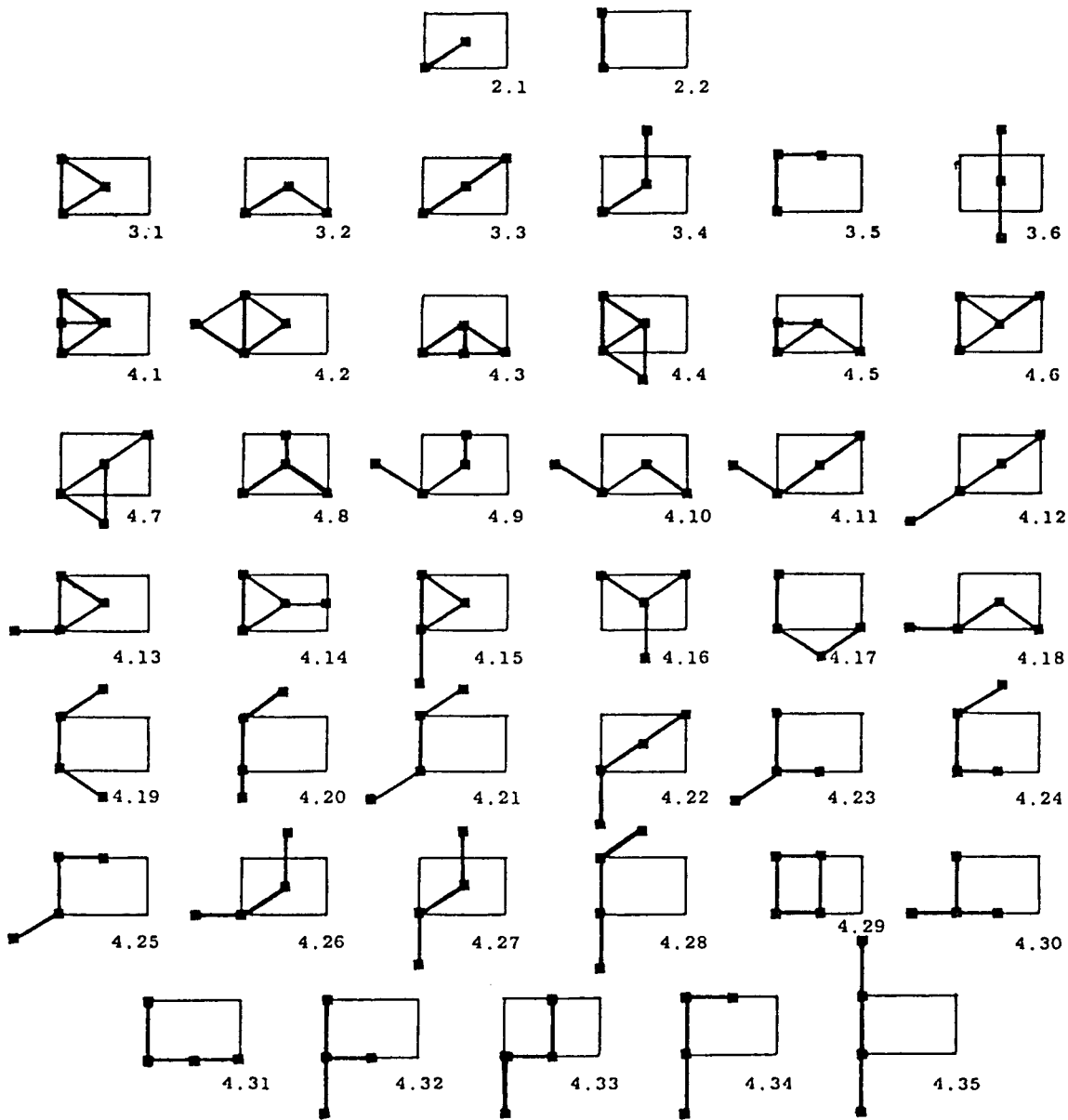
Figure 1. Crystallographically distinct close-packed 2, 3 and 4 vacancy clusters in BCC crystals projected onto the (110) plane

E are irrelevant. Although the FS potential has almost the same range as the J_0 potential, the effect of higher bonds contributes significantly to the energy values. That is why the binding energies of all the clusters involving higher bonds are distinct. Two pairs of clusters 4.21, 4.22 and 4.32, 4.33 have the same binding energies in the case of pair potential calculations, while the many body potential gives distinct binding energies for all of them. The general effect is that the binding energy increases with the compactness of the cluster. In all the calculations, it is observed

that the neighbouring atoms relax over short distances to reach their equilibrium postitions. However, none of the initial clusters collapse into a new distinct form.

Discussion

The prime aim of this study was to use the many body FS potential for the vacancy clusters in BCC iron and get information about their binding energies. The relaxed structures and energies of 2, 3 and 4 vacancy clusters have been obtained. Examination of the atomic structures of the

two di-vacancies reveals that the four atoms clustered around a B-type axis relax far more than the six atoms clustered around an A-type axis, and hence give a lower formation energy and therefore a higher binding energy. The present results of binding energies of the clusters are generally higher than the earlier ones. The type B di-vacancy has 22% higher binding energy while the type A di-vacancy has only 5% higher than their respective pair potential values. Thus, under FS calculations, the type B di-vacancy is even more strongly bonded than the type A di-vacancy. This effect is dominant in all the results, and clusters with the greater number of B bonds have the larger binding energies.

In the case of pair potentials, third and higher (C, D, E,...) bonds have little significance. On the other hand, the many body potential has a long range effect and all the higher order bonds contribute towards the binding energy of a cluster. Due to this fact, two pairs of tetra-vacancy clusters 4.20, 4.21 and 4.32, 4.33, which have exactly the same binding energies under J_0 potential, are clearly differentiable here, and, in fact, all the clusters simulated have distinct binding energy values.

A detailed examination of Table 1 reveals that the binding energies of all the clusters are higher with many body potential as compared to the pair potential calculations with the exception of clusters 3.2, 4.8, 4.9 and 4.10. In these cases, the results have even lower values than the earlier ones. This is due to the absence of B bonds and the presence of C bonds. In FS potential, the C bonds are strongly repulsive while B bonds are strongly attractive. Thus, the clusters with a higher number of B bonds and a lower number of C bonds are the most stable ones.

The binding energies of clusters clearly depend on the reliability of the computational procedure adopted and the potential used. As far as the computing techniques are concerned, it is found that they incorporate the newly developed FS potential, handle the structures with ease and allow them to relax satisfactorily to plausible equilibrium configurations. Thus FS potential can be relied upon to achieve acceptable results for α-iron.

Acknowledgements

References

1. Allnatt, A. R. and Allnatt, E. L. Crystall Lattice Defects, 5, 181, (1974).

2. Crocker, A. G. *Phil. Mag.* 32, 379, (1975).

3. Crocker, A. G. Crystal Lattice Defects, 7, 239, (1978).

4. Ahmad, S. A., Crocker, A. G. and Faridi, B. A. *Phil. Mag.*, A, 48, 31, (1983).

5. Malik, A. Q. and Crocker, A. G. *Ibid*, 51, 551, (1985).

6. Johnson, R. A. *Phys. Rev.*, A, 134, 1329, (1964).

7. Gorecki, T. Z. *Metallk.*, 65, 426, (1974).

8. Dederiches, P. H., Lehmann, C., Schober, H. R., Scholz, A. and Zeller, R., *J. Nucl. Mater.*, 69, 176, (1978).

9. Finnis, M. W. and Sinclair, J. E. *Phil. Mag.*, A, 50, 45, (1984).

10. Finnis, M. W. and Sinclair, J. E. *Ibid*, A, 53, 161, (1986).

11. Matthai, C. C. and Bacon, D. *Ibid*, 52, 1, (1985).

12. Harder, J. M. and Bacon, D. *Ibid*, A, 54, 651, (1986).

13. Harder, J. M. and Bacon, D. *Ibid*, A, 58, 165, (1988).