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COMPUTATIONAL ENUMERATION OF POINT DEFECT CLUSTERS IN DOUBLE- LATTICE CRYSTALS

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Abstract

The cluster representation matrices have already been successfully used to enumerate close-packed vacancy clusters in all single-lattice crystals [1, 2]. Point defect clusters in double-lattice crystals may have identical geometry but are distinct due to unique atomic postions enclosing them. The method of representation matrices is extended to make it applicable to represent and enumerate the point defect clusters in multi-lattice crystals as well. A computational procedure based on family representation matrices is developed and applied to the hexagonal close-packed structure.

Introduction

Brody and Meshii [3], Crocker [4] and other research workers have developed various methods to identify distinct close-packed point defect clusters in crystals. These are confined to cubic crystals and therefore could not be adopted for double-lattice structures. The concept of cluster representation matrices have been developed and applied to enumerate vacancy and vacancy-solute mixed clusters in all single crystals by Ahmad et al. [1] and Malik et al. [2]. When this method is applied to double-lattice crystals discrepancies arise due to the fact that there are some vacancy clusters which have exactly the same geometry but are distinct due to the unique atomic positions surrounding them. To illustrate this problem two distinct h.c.p. trivacancy clusters having identical geometric shapes are shown in Fig. 1 (a and b).

Among the other methods, the most reliable one is due to Crocker [5]. In this method the clusters are enumerated by sketching and visual inspection of all of their possible orientations (variants). The method is tiresome and may give unsatisfactory results for bigger clusters. As the sketching procedure [4] cannot be adopted for computational treatment of the problem, therefore a numerical method is necessary for the fast and accurate enumeration of the distinct vacancy clusters in double-lattice crystals. The present note describes the extension of the matrix representation procedure to enumerate the clusters in multi-lattice crystals.

Keywords: Vacancy Clusters, Point Defect

Family Representation Matrix

An n-point cluster having m community points (those having first neighbour relation with at least two points of the cluster) is called a family as a whole. Let all n points of a cluster itself and m those of its community points be labelled by positive integers i such that $i \le n$ and $n < i \le (n+m)$ respectively. The (n+m)x(n+m) square array of distances R_{ij}, between points i and j, is then known as a family representation matrix F_{ij} of the cluster:

$$
F_{ij} = \left[\begin{array}{ccc|cc}
0 & R_{12} & R_{1n} & R_{1(n+1)} & R_{1(n+m)} \\
R_{21} & 0 & R_{2n} & R_{2(n+1)} & R_{2(n+m)} \\
- & - & - & - & - \\
- & - & - & - & - \\
R_{n1} & R_{n2} & 0 & R_{n(n+1)} & R_{n(n+m)} \\
\hline
R_{(n+1)1} & R_{(n+1)2} & R_{(n+1)n} & 0 & R_{(n+1)(n+m)} \\
- & - & - & - & - \\
- & - & - & - & - \\
R_{(n+m)1} & R_{(n+m)2} & R_{(n+m)n} & R_{(n+m)(n+1)} & 0
\end{array}\right]
$$

Clearly this matrix is symmetric and has zero elements along its principal diagonal. The matrix F_{ij} can be divided into four submatrices having their own representative properties. The top left (n x n) square matrix R_{ij} is the well-known cluster representation matrix [1]. The bottom right (m x m) square array could be named as Community Representation Matrix C_{ij} because this gives the relationship among the community points. The remaining two (n x m) and (m x n) matrices are mutually transpose and tabulate the relationship between cluster and those of the community points and thus are named as Relation Matrices.

There are n (n-1)/2 elements R_{ij}, $1 \le i < j \le n$, which occupy the upper/ lower triangle of the cluster representation matrix. Similarly m(m-1)/2 elements C_{ij}, $(n+1) \le i < j \le (n+m)$, occupy the upper/lower triangle of community representation matrix. It is convenient to write the elements in the form of a single row or cluster representation vector C_α. For example, for n=3 and m=4 $R_\alpha = (R_{12}, R_{13}, R_{23})$ and

$$C_\alpha = (C_{45}, C_{46}, C_{47}, C_{56}, C_{57}, C_{67}).$$

As there are n-points in a cluster having m community points that can be labelled in any order, there are in general n! and m! possible representation matrices for a given configuration. These matrices are related by coordinated interchanges of rows and corresponding columns. It is necessary, of course, to select one for each to characterize the cluster. The characteristic choice is the matrix corresponding to the cluster representation vector ${}^{C}R_\alpha$ and community representation vector ${}^{C}C_\alpha$ in which as for as possible short lengths take the precedence [1].

For the h.c.p. divacancies shown in Fig. 1, (c&d) the characteristic representation and community representation matrices are:

$$R^{c}_{ij} = \begin{bmatrix} O & A \\ A & O \end{bmatrix} \qquad R^{d}_{ij} = \begin{bmatrix} O & A \\ A & O \end{bmatrix}$$

$$C^{c}_{ij} = \begin{bmatrix} O & A & A & D \\ A & O & C & B \\ A & C & O & B \\ D & B & B & O \end{bmatrix} \qquad C^{d}_{ij} = \begin{bmatrix} O & A & B & D \\ A & O & D & B \\ B & D & O & A \\ D & B & A & O \end{bmatrix}$$

where A, B, C, - - - represent the lst, 2nd, 3rd, - - - nearest-neighbour distances respectively The corresponding characteristic cluster and community representation vectors are:

$${}^{C}R^{C}_{\alpha} = A; \qquad {}^{C}C^{C}_{\alpha} = AADCBB$$

$${}^{C}R^{d}_{\alpha} = A; \qquad {}^{C}C^{d}_{\alpha} = ABDDBA$$

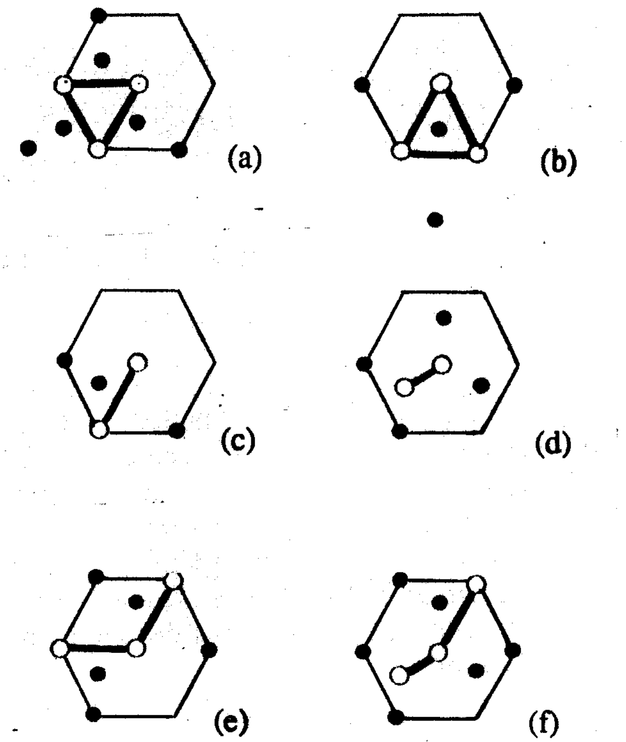

Figure 1. Cluter of 2,3 points on h.c.p. lacttice. open 7 solid circles denote the cluster and community points respectively

True representation vector T_α is formed by writing the cluster representation vector followed by community representation vector in the same parenthesis pair as:

$$T^{c}_{\alpha} = (A; AADCBB)$$

$$T^{d}_{\alpha} = (A; ABDDBA).$$

As a further example of the appliction of this method to the identification of h.c.p clusters shown in Fig. 1 (e & f) have the characteristic representation matrices:

$$R^{e}_{ij} = \begin{bmatrix} 0 & A & A \\ A & 0 & D \\ A & D & 0 \end{bmatrix} \qquad R^{f}_{ij} = \begin{bmatrix} 0 & A & A \\ A & 0 & D \\ A & D & 0 \end{bmatrix}$$

$$C^{e}_{ij} = \begin{bmatrix} O & A & A & B & B & D & D \\ A & O & C & A & E & D & B \\ A & C & O & E & A & D & B \\ B & A & E & O & C & A & D \\ B & E & A & C & O & A & D \\ D & D & D & A & A & O & D \\ D & B & B & D & D & D & O \end{bmatrix} \qquad C^{f}_{ij} = \begin{bmatrix} O & A & A & A & D & D & D \\ A & O & B & C & D & A & B \\ A & B & O & B & A & D & F \\ A & C & B & O & D & E & B \\ D & D & A & D & O & B & D \\ D & A & D & E & B & O & A \\ D & B & F & B & D & A & O \end{bmatrix}$$

n.j	Solution set corresponding to: Cluster Representation Matrix	Solution set corresponding to: Community Representation Matrix
3.1	7071 7071 7071	4883 4883 4883 5342 5342
3.2	7071 7071 7071	3501 3501 3501 3501 3501 3501 3912 3912 3912
3.3	7071 7071 7071	3775 3775 4067 4410 4410 4317 4502
3.6	7071 7071 7753	3870 3870 4103 4103 4138 4431 4694
3.7	7071 7071 7753	3784 3822 3912 4215 4428 4519 4554
4.2	5662 5662 5996 5996	3244 3244 3284 3284 3330 3498 3498 3508 3508 4031
4.3	5662 5662 5996 5996	3713 3927 4138 4157 4316 4394 4684
4.5	5415 5415 6491 6419	3243 3243 3243 3243 3443 3443 3566 3566 3666 3666
4.6	4515 4515 6491 6419	2580 2714 3586 3794 3795 3848 3989 4211 4344
4.8	5522 5739 6059 6361	3602 3667 3719 3735 3763 3805 4419 4437
4.9	5522 5739 6059 6361	2636 2937 3208 3486 3509 3534 3697 3749 3883 3936
4.10	5522 5739 6059 6361	2891 3250 3415 3576 3615 3814 3909 4042 4430
4.13	5752 5752 5817 6533	2871 2871 2983 2983 3113 3505 3505 3583 3583 3583 3583
4.14	5752 5752 5817 6533	3126 3366 3430 3549 3558 3718 3831 4077 4267
4.16	5472 5794 6054 6853	3606 3643 3643 3748 3909 4077 4260 4260
4.17	5472 5794 6054 6853	2603 2780 2780 2933 2933 3044 3101 3101 3309 3309 3783 3944
4.18	5472 5794 6054 6853	2747 2786 2952 3212 3513 3629 3829 3832 3879 4185
4.26	5615 5812 6062 6232	3243 3301 3558 3600 3690 3801 3844 3894 3917
4.27	5615 5812 6062 6232	3113 3334 3699 3969 4136 4165 4276 4673
4.28	5615 5812 6062 6232	2918 3214 3509 3577 3628 3773 3987 4053 4428
4.31	5772 5775 6061 6588	3026 3198 3380 3666 3908 3929 3939 3962 4051
4.32	5772 5775 6061 6588	3083 3124 3146 3217 3226 3413 3698 3797 3968 4061
4.41	5958 5958 6004 6004	2735 2735 3229 3229 3229 3229 3610 3610 4587 4982
4.42	5958 5958 6004 6004	3154 3154 3154 3154 3401 3401 3550 3550 3866 4044
4.43	5958 5958 6004 6004	3161 3161 3335 3335 3587 3587 4185 4499 4587
4.45	5876 5876 6306 6306	2726 2895 3224 3375 3464 3560 3748 3826 3885 3975
4.46	5876 5876 6306 6306	3001 3381 3459 3550 3873 3877 3899 3909
4.48	5795 5795 6527 6527	3154 3161 3161 3207 3207 3273 3561 3561 4152 4359
4.49	5795 5795 6527 6527	3154 3359 3370 3542 3572 3577 3731 4245 4388
4.52	5903 6014 6030 6660	2675 2678 3015 3015 3156 3171 3171 3678 3678 4033 4244
4.53	5903 6014 6030 6660	2700 2921 2936 3071 3129 3217 3270 3503 3630 3870 4095
4.54	5903 6014 6030 6660	2439 3058 3058 3110 3110 3256 3325 3622 3622 3745 3790

Table 1- Results for pairs and triplets of n-points clusters, in h.c.p. crystal, having identical geometry. multiplied by 10^4

As both of the clusters have exactly the same geometric shape therefore they have the same cluster representation vector ${}^{C}R^{e}_{\alpha} = {}^{C}R^{f}_{\alpha} = AAD$. However, the community representation vectors

${}^{C}C^{e}_{\alpha}$=AABBDDCAEDBEADBCADADD and

${}^{C}C^{f}_{\alpha}$=AAADDBCDABBADFDEBBDA are distinct. Thus $T^{C}_{\alpha} = ({}^{C}R^{e}_{\alpha}; {}^{C}C^{e}_{\alpha})$ and $T^{f}_{\alpha} = ({}^{C}R^{f}_{\alpha}; {}^{C}C^{f}_{\alpha})$ are distinct beyond their fifth elements. True representation vectors provide a comprehensive method of enumeration of point clusters in double-lattice crystals.

The more simple and efficient computational method based on representation matrices [6] can also be extended for double-lattice structures. The cluster representation and community representation matrices are converted into its augmented form by adding a column vector whose elements are obtained by taking square root of the sum of square of the corresponding row elements. This forms two systems of linear equations. The ordered solutions of both the systems are compared one by one for the recognition of distinct cluster configurations. For the purpose of cluster enumeration one has to compare the second sets of solutions of the clusters only if the first sets happen to be identical. The solution sets of clusters shown in Fig. 1 (c & d), by substituting the numeric values of A, B, C, - - - are x^{c} = (0. 1, 0. 1; 0.5547, 0. 5547, 0.5957, 0.6031) and x^{d} = (0.1, 0.1; 0.5908, 0.5908, 0.5908, 0.5908). Similarly x^{e} = (0.707, 0.707, 0.775, 0.387, 0.387, 0.410, 0.410, 0.414, 0.443, 0.469) and x^{f} = (0.707,0.707,0.775; 0.378, 0.382, 0.391, 0.422, 0.422, 0.452, 0.455)

Results and Discussion

The method described above is applied to recognize distinct close-packed vacancy clusters in h.c.p. crystals. Results for groups of tri-and tetra-vacancy clusters, which are not distinguishable by cluster representation matrix procedure, are presented in Table 1. The cluster classification number is taken from reference [5]. The penta-vacancy clusters are enumerated to be 458.

The present method overcomes the ambiguities arising in recognizing the clusters having identical geometry. Although the method of true representation vectors solves the problem of cluster enumeration, however it is time consuming as it has to consider all n! equivalent (n x n) cluster representation and m! equivalent (m x m) community representation matrices for an n point cluster having m community members. In the case of numerical method any one of the n! and m! representation matrices can be used to recognize a cluster. Therefore considerable computational time, as compared to method of true representation vectors, is saved.

Several conclusions can be drawn from the results presented in Table 1. It is possible, for example, to predict the symmetry of a cluster from its solution set because its equivalent or identical viewpoints have always the same numerical values. The same is true for community points as well. It is interesting to note that cluster configuration 4.3 has two pairs of identical view points but no two of the seven community points have identical situation.

For the fast enumeration of clusters, of a certain size, only community representation matrix considerations are sufficient. However, to deduce the full clustral properties one has to take both of the representation matrices. The method is applicable to crystal structure of any complexity.

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