The properties of an ordering solid solution are substantially dependent on the long-range and short-range order parameters; a method is given for representing a binary solid solution as a set of cluster components whose short-range order parameters are incorporated out to the second coordination sphere. The scheme is illustrated via the lattice parameter and Debye temperature for Ti–Mo alloys (bcc lattice) and via the magnetic moment of Fe–Pd alloys (fcc lattice). The method allows one to describe nonmonotonic composition–property relationships and to define the values of properties for ordered structures.

A general scheme has been described [1] for incorporating the short-range order of a multicomponent solid solution for an arbitrary number of coordination spheres; the solid solution is then characterized via a matrix containing $n^2$ columns and $m+1$ rows, where $n$ is the number of components in the solution and $m$ is the number of coordination spheres.

A binary solution $A_cB_{1-c}$ is described by the following matrix when one coordination sphere is incorporated:

$$
\begin{pmatrix}
A & B & A & B \\
c & 0 & 0 & 1-c \\
\left(\frac{p_1}{2} \right) & \frac{p_1}{2} & \frac{p_1}{2} & 1-c - \frac{p_1}{2}
\end{pmatrix},
$$

(1)

where $p_1$ is the probability of formation of a first-order $A-B$ pair.

The region of existence of the solid solution (in terms of the variables $c$ and $p_1$) is represented by the triangle in Fig. 1a, whose vertices correspond to three cluster components. The line I–III–II in Fig. 1a corresponds to the maximum possible $p_1(c)$, the course of $p_1^{\text{max}}(c)$ for a particular lattice may differ from I–III–II.

For instance, $p_1(1/2)$ for a bcc solid solution may take the value 1 (ordering of $\beta$-brass type), whereas $p_1(1/2) = 1$ is essentially impossible for a solid solution with an fcc lattice.

We consider a solid solution $A_cB_{1-c}$ with a bcc lattice; the nearest neighbors in that case are in different sublattices, so $p_1(c)$ will equal $p_1^{\text{max}}(c)$ if the $A$ atoms initially fill one of the two sublattices ($c < 0.5$) and only then fill the other ($c > 0.5$); we then have

$$
p_1^{\text{max}}(c) = 2c \quad \text{for} \quad c \leq 1/2,
$$

$$
p_1^{\text{max}}(c) = 2(1-c) \quad \text{for} \quad c \geq 1/2.
$$

(2)

The form of $p_1^{\text{max}}(c)$ is then represented by I–III–II in Fig. 1a, while the points I, II, and III correspond to three cluster components:

$$
\begin{pmatrix}
0 & 0 & 1 \\
0 & 0 & 0 \\
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 1 & 2 \\
1 & 2 & 2
\end{pmatrix},
$$

(3)

Clusters I and II are the pure $B$ and $A$ components, while cluster III is the $A_{1/2}B_{1/2}$ equimolar alloy ordered in the style of $\beta$-brass.
Fig. 1. Regions of definition of the matrix of (1): a) bcc lattice; b) fcc lattice.

TABLE 1. Decomposition of the Matrix for the Solution of (1) into Cluster-Component Matrices of (6) for a Binary Solution with an fcc Lattice Incorporating only One Coordination Sphere

<table>
<thead>
<tr>
<th>№</th>
<th>I</th>
<th>II</th>
<th>III</th>
<th>IV</th>
<th>V</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1 - 2 (p_l)</td>
<td>6(p_l) - 8c</td>
<td>6c - 3(p_l)</td>
<td>2c - (p_l)</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1 - 2(p_l)</td>
<td>3(p_l) - 2c</td>
<td>(3p_l) - 2c</td>
<td>(8/3) c - 2(p_l)</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>1 - (p_l) - (2/3) c</td>
<td>(3p_l) - 2c</td>
<td>(3p_l) - 2c</td>
<td>(8/3) c - 2(p_l)</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>1 - (p_l) - (2/3) c</td>
<td>2(p_l)</td>
<td>(3/2) (p_l)</td>
<td>(c - (3/4) (p_l)</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>1 - (c)</td>
<td>(3/2) (p_l)</td>
<td>(3/2) (p_l)</td>
<td>(c - (3/4) (p_l)</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>(8/3) (-) (2(p_l)</td>
<td>(3p_l) + 2c - 2</td>
<td>(1/3) + (2/3) c - (p_l)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>(1 - (p_l)</td>
<td>(2(p_l)</td>
<td>(2(p_l)</td>
<td>(c - (3/2) (p_l)</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>(2 - 2c - (p_l)</td>
<td>(6 - 6c - 3(p_l)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The matrix of (1) splits up unambiguously into these components:

\[
\begin{pmatrix}
  c & 0 & 0 & 1 - c \\
  c - \(p_l\) & \(p_l\) & \(p_l\) & 1 - c - \(p_l\)
\end{pmatrix}
= \left(1 - c - \(p_l\) \right) \begin{pmatrix} 0 & 0 & 0 & 0 \end{pmatrix} + \nonumber \\
+ \left( c - \(p_l\) \right) \begin{pmatrix} 1 & 0 & 0 & 0 \end{pmatrix} + \(p_l\) \begin{pmatrix} 1/2 & 0 & 0 & 1/2 \end{pmatrix}.
\]

We now consider a solid solution \(A_\alpha B_1 - c\) with an fcc lattice; the nearest neighbors in that case lie in different sublattices, and \(p_l(c)\) will equal \(p_l^{\text{max}}(c)\) if the A atoms fill each of the sublattices in turn. Then

\[
\begin{align*}
p_l^{\text{max}}(c) &= 2c, & \text{for } 0 \leq c \leq 0.25, \\
p_l^{\text{max}}(c) &= \frac{1 + 2c}{3}, & \text{for } 0.25 \leq c \leq 0.5, \\
p_l^{\text{max}}(c) &= \frac{3 - 2c}{3}, & \text{for } 0.5 \leq c \leq 0.75, \\
p_l^{\text{max}}(c) &= 2(1 - c), & \text{for } 0.75 \leq c \leq 1.
\end{align*}
\]

The region of existence of the solid solution is represented by the pentagon of Fig. 1b, whose vertices correspond to five cluster components:

\[
\begin{pmatrix} 0 & 0 & 0 & 1 \\
 0 & 0 & 0 & 1
\end{pmatrix}, \begin{pmatrix} 1/4 & 0 & 0 & 3/4 \\
 0 & 1 & 1 & 1
\end{pmatrix}, \begin{pmatrix} 1/2 & 0 & 0 & 1/2 \\
 1 & 1 & 1 & 1
\end{pmatrix}, \begin{pmatrix} 3/4 & 0 & 0 & 1/4 \\
 1 & 1 & 1 & 1
\end{pmatrix}, \begin{pmatrix} 1/2 & 0 & 0 & 1/2 \\
 2 & 4 & 4 & 2
\end{pmatrix}, \begin{pmatrix} 3/4 & 0 & 0 & 1/4 \\
 1 & 1 & 1 & 1
\end{pmatrix}, \begin{pmatrix} 1/2 & 0 & 0 & 1/2 \\
 2 & 4 & 4 & 2
\end{pmatrix}, \begin{pmatrix} 3/4 & 0 & 0 & 1/4 \\
 1 & 1 & 1 & 1
\end{pmatrix}, \begin{pmatrix} 1/2 & 0 & 0 & 1/2 \\
 2 & 4 & 4 & 2
\end{pmatrix}.
\]