Solubility of Boron and Carbon in Alloys \((\text{Fe Me})_2 \text{BC}, (\text{Me} = \text{Fe, Cr, Mn, Al etc.})\)

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**Abstract**

The calculation of solubility of Boron and Carbon in alloys \((\text{Fe Me})_2 \text{BC}, (\text{Me} = \text{Fe, Cr, Mn, Al etc.})\) is made. A modified model Hume-Rothery of crystal is accepted. A method of configuration that takes into account all possible configurations of atoms Fe, Me around atoms of Boron and Carbon is used.

Formulas determining solubility of Boron and Carbon alloys dependent on temperature and concentration of components of Fe, Me and energetic constants and those determining mutual influence of solubility of Boron and Carbon in alloy are obtained. The formulas assume extreme temperature dependence of solubility.

In recent times attention of scientists has been attracted to borides because of their specific properties such as high hardness, refractoriness, resistance to creep. Efficiently alloyed Boron – containing alloys are widely used in surface coating. They are wear resistant and their performances are not worse than those of rare expensive alloys. Researches of finite solubility of admixtures in iron-boride is of great scientific and practical interest as it allows to estimate concentration and temperature areas of existence of continuous solid solutions.

In the paper calculation of solubility of Boron and Carbon in alloys \((\text{Fe Me})_2 \text{BC}, (\text{Me} = \text{Fe, Cr, Mn, Al etc.})\) is made.

Free energy of an alloy is calculated for a crystal lattice in a modified Hume-Rothery model [1]. A method of configuration that takes into account all possible configurations of Fe, Me atoms around of B and C is used [2].

Fig. 1 shows an elementary crystal cell which has lattice sites of four types for atoms of Fe, Me, B and C correspondingly. Each of the lattice sites of the second and the fourth types form a bodycentered tetrahedral (BCT) lattice. These lattices are inserted one into another as it is shown on Fig. 1 (a) and (b).
The sites of the first and third types distribute in layers (Fig. 1, c).
Atoms of Boron and Carbon replacing lattice sites of the second and the fourth types are located in the centre of the tetraheds formed by atoms of iron and metal Me.

Figure 1.

The elementary cell of crystal (Fe Me)₂ BC in modified model Hume-Rothery.
(a) The atoms Fe and Me tetrahedron surround the sites for atoms B.
(b) The atoms Fe and Me tetrahedron surround the sites for atoms D.
(c) The layers distribution of sites crystal of different type as Z-axis.

- The sites of first type for Fe atoms.
- The sites of second type for B atom.
- The sites of third type for atoms Me = Cr, Mn, Al etc.
- The sites fourth type for atoms D = B, C, N, H, Si etc.
Further there is examined an alloy which does not have an atomic order either in distribution of atoms of iron and metal Me or atoms of Boron and Carbon. Besides, interaction of couples Fe Fe, Fe Me, Me Me can be omitted in the calculation as the corresponding summands of free energy disappear at it minimization. Some of the lattice sites which are true for atoms of Boron and Carbon are vacant and at solution of Boron and Carbon new atoms occupy vacant lattice sites.

The calculation of free energy of an alloy gives the formula

\[
F = - \sum_{i=0}^{4} (N_{B_i} V_{B_i} + N_{C_i} V_{C_i}) - \\
- \frac{1}{N} \sum_{i=0}^{4} \left[ N_{B_i}^2 (V_{BB} + 2V_{BB'}) + N_{C_i}^2 (V_{CC} + 2V_{CC'}) + 2N_{B_i}N_{C_i} (V_{BC} + 2V_{BC'}) \right] - \\
- kT \sum_{i=0}^{4} \left[ Q_i \lambda_i n_i - N_{B_i} \lambda_i n_{B_i} - N_{C_i} \lambda_i n_{C_i} - (Q_i - N_{B_i} - N_{C_i}) \lambda_i n(Q_i - N_{B_i} - N_{C_i}) \right] ,
\]

where \(N_{\alpha_i}\) are the numbers of \(\alpha = B,C\) atoms with \(i\) - configuration of Fe and Me atoms; \(V_{\alpha_i} = V_{\alpha_i}(r), V'_{\alpha_i} = V_{\alpha_i}(r')\) are the energy of atoms \(\alpha\) with \(i\) – configuration in the distance \(\rho = \frac{c}{2}, r' = \frac{a}{\sqrt{2}}\); \(V_{\alpha\beta}, V'_{\alpha\beta}\) are the interaction energy of atomic pairs \(\alpha, \beta = B,C\); \(Q_i\) is the number of sites for \(B,C\) atoms with \(i\) - configuration.

Minimizing free energy at \(N_{B_i}\) and \(N_{C_i}\) we find the equilibrium concentration equations or solubility of \(B\) and \(C\) in the alloy

\[
b = D_1 \exp \frac{2[b(V_{BB} + 2V'_{BB}) + c(V_{BC} + 2V'_{BC})]}{kT} \left( f \exp \frac{V_{BF}}{kT} + m \exp \frac{V_{BM}}{kT} \right)^4 ,
\]
\[
c = D_2 \exp \frac{2[b(V_{BC} + 2V'_{BC}) + c(V_{CC} + 2V'_{CC})]}{kT} \left( f \exp \frac{V_{CF}}{kT} + m \exp \frac{V_{BM}}{kT} \right)^4 ,
\]

where \(D_1, D_2\) are the \(B\) and \(C\) atoms activity, \(b, c, f, m\) are the atomic concentration of \(B, C, Fe, Me\) components.

The obtained above formulas (2) and (3) determine solubility of Boron and Carbon in dependence on temperature and concentration of the Fe and Me components as well as interdependence of Boron and Carbon solubility in an alloy.

It is easy to get persuaded that the type of mutual dependence of the solubility of one of the \(B\) and \(C\) components on the solubility of the other is determined by numerical values and energy
signs $V_{BC}, V_{BC}^\prime$. At $V_{BC}, V_{BC}^\prime > 0$ when there are forces of attraction between atoms of Boron and Carbon, Carbon admixture promotes the Boron solubility and vice versa at $V_{BC}, V_{BC}^\prime < 0$ in the case of forces of repulsion existing between atoms of Boron and Carbon. Carbon admixture prevents from the Boron solubility. The second case corresponds to the experimental data [3].

Bibliography