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# CLUSTERS IN CARBON MARTENSITE. PART I. MARTENSITE IN THERMODYNAMIC EQUILIBRIUM

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An original method of evaluation of the cluster population in carbon martensite has been developed [1]. Using this method it was shown that the Kurdiumov's model of a carbon redistribution within the different octahedral site sublattices can quantitatively account for both observed normal and abnormal tetragonality in carbon martensite. It was also shown that an existence of the internal strains in martensite constitutes a necessary and sufficient condition for the energetic preference of tetrahedral site over the cubic one. The presence of the residual tetragonal distortion in the quasi-cubic phase of κ- martensite is associated with the presence of the mixed clusters formed of the atoms belonging to $O_c$ sublattice as well as to remaining ones.

The long - range ordering parameter $\eta$ is associated with the mean carbon concentration on sublattice $C(O_a)$, $C(O_b)$ and $C(O_c)$ by the following relations :

$$C(O_a) = C(O_b) = C(1-\eta)/3 \qquad (1)$$
$$C(O_c) = C(1+2\eta)/3$$

On the other hand, the internal energy, may be expressed as:

$$U = N \Sigma V_n C_n \qquad (2)$$

where: $V_n$ - binding energy per atom,
$C_n$ - probability that a given atom belongs to cluster n
N - total number of iron atoms.

Taking into account eq. (1) and the law of conservation of the total number of particles in the sublattices, we obtain:

$$\Sigma_{(\alpha)}C_\alpha + \Sigma_{(\gamma)} (a_\gamma /n_\gamma ) C_\gamma = C(1+2\eta)/3 \qquad (3)$$
$$\Sigma_{(\beta)} C_\beta + \Sigma_{(\gamma)} (b_\gamma /n_\gamma ) C_\gamma = C(1+2\eta)/3$$

where the subscript $\alpha$ labels the clusters composed of the atoms located in $O_C$ sites, while the subscript $\beta$ - labels the clusters composed of atoms located in $O_a$ or $O_b$ sites. The $\gamma$ subscript labels the mixing of the atoms in n-particle clusters with $a_\gamma$ atoms in $O_c$ and $b_\gamma$ atoms in $O_a$ or $O_b$ sublattices.

The entropy S can be expressed as:

$$S = S_L + S_{sh} \qquad (4)$$

where $S_L$ is the entropy connected with long-range ordering, $S_{sh}$ the entropy connected with short-range ordering. Taking into account eq. (1), the entropy $S_L$ can be expressed as:

$$S_L = kN[C(1+2\eta)/3 \ln C(1+2\eta)/3 + (1-C/3 -2C\eta) \ln C(1+2\eta)/3+2C(1-\eta)/3\ln C(1-\eta)/3+2(1-C/3+C\eta/3)\ln(1-C/3+C\eta/3)] \qquad (5)$$

The entropy $S_{sh}$, may be obtain in the form:

$$S_{sh} = -kN[\Sigma_{(\alpha)}R_\alpha \ln(1-C_\alpha/R_\alpha) + 2\Sigma_{(\beta)}R_\beta \ln(1-C_\beta/R_\beta)+ \Sigma_{(\gamma)}R_\gamma \ln(1-C_\gamma/R_\gamma ) +\Sigma_{(\alpha)}C_\alpha \ln C_\alpha/(R_\alpha-C_\alpha)+2\Sigma C_{(\beta)} \ln C_\beta/(R_\beta-C_\beta) +\Sigma_{(\gamma)}C_\gamma \ln_\gamma C_\gamma/(R_\gamma-C_\gamma)] \qquad (6)$$

where $R_{\alpha,\beta,\gamma}$ are numbers of possibilities of rotations transforming a given cluster into another one. Concentrations $C_\alpha$, $C_\beta$ and $C_\gamma$ must satisfy the equation (3). For equilibrium state, from the condition of minimum free energy, we have a system of equations from which all order parameters can be derived. Omitting technical details of calculations we obtain:

$$C_\alpha /(R_\alpha - C_\alpha) = N_1 \exp(-V_\alpha/kT)$$
$$C_\beta /(R_\beta - C_\beta) = N_2 \exp(-V_\beta/kT) \qquad (7)$$
$$C_\gamma /(R_\gamma - C_\gamma) = (N_1)^{a\gamma/n\gamma}(N_2)^{b\gamma/n\gamma} \exp(-V_\gamma/kT)$$

where normalization constants $N_1$ and $N_2$ can be found numerically using jointly eq.(7) and eq.(3).

REFERENCES:

[1]. L. Dąbrowski: *Metall. Mater. Trans.* -in press.