ANALYSIS AND INTERPRETATION OF DATA ON THE EVOLUTIONARY DEVELOPMENT OF DISPERSED SYSTEMS

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We discuss questions concerning the application of systems analysis to alloys containing a dispersed phase. The development of such dispersed systems takes on the form of self-development of an ensemble of polydispersed microparticles distributed in the matrix phase, which we can evaluate from data on analysis of the transformation of their size distributions over time. For the example of vanadium steel containing dispersed carbide phase (cementite + VC carbides), we illustrate the procedure for establishing a correlation between the indices of the transformation of the experimental histograms over time for enlargement of the Fe3C microparticles in the alloy and the internal processes (within the volume) causing such transformations, and also the interpretation of the data obtained and the characteristic features of application of the developed method to a system analysis of the evolution of microparticles of dispersed systems.

Solid dispersed systems (for example, metallic alloys hardened by dispersed phases) are characterized by excess free energy, mainly as a result of the extended phase interface surface. Thermal energy input from outside the system is transformed to system entropy, i.e., entropy is produced in the system, as a result of dissolution of the smallest particles and growth of the larger particles. The excess free surface energy of the dispersed phase is liberated and the structural state of the material of the medium at the interphase boundary becomes closer to equilibrium. Self-consistency of the diffusion field of material fluxes of the dispersed phase in the medium (the matrix phase) determines the existence of each microparticle at any specified moment of time. In turn, the material of the medium, interacting with the dispersed particles, is the carrier of the future forms of organization of the dispersed system as it moves from state of instability, which also decides the predeterminacy of the evolution of the processes, the choice of the life line for the system itself.

A general characteristic of a dispersed system is that the size distribution of the microparticles undergoes a continuous transformation in its evolutionary development, which may serve as important information about the nature of the intrasystem processes. We solve the analogous problem in this paper for the example of the evolution of microparticles of cementite phase in vanadium steel. The information obtained may be useful in creating a technique for analysis and study of evolving dispersed systems.

Results of System Analysis and Discussion. Below we present an analysis of data on the size distribution of Fe3C microparticles, obtained upon isothermal heating of vanadium steel (97.2% Fe; 1.37% C; 0.75% V; 0.35% Mn, and 0.33% Si) at a temperature of 750°C [1]. With the goal of obtaining a finely dispersed phase, the steel samples were heated up to 1100°C, held at this temperature for 10 min, and after quenching in water they were tempered for three hours at 620°C. After additional heating of the samples for one hour at 750°C, we did an initial analysis of a dispersed phase consisting of microparticles of cementite Fe3C and a special VC carbide (V4C3), distributed in an austenitic matrix phase. In [1], data are presented on the transformation of the experimental distributions: histograms for the system of microparticles of cementite phase over the isothermal holding time of steel at 750°C.

The characteristics of the experimental size distributions of Fe3C microparticles are presented in Table 1. The preliminary two-dimensional surface distributions of microparticles n_r were recalculated as three-dimensional interior distributions using formula (7) in [2], then we determined the total number of microparticles per unit volume of the steel N, their average radius \( \bar{r} \), the modal size \( r_m \), the upper size limit (the range of the distribution) \( r_g \), its asymmetry coefficient.
TABLE 1. Characteristics of Size Distributions of Fe₃C Microparticles after Isothermal Tempering at 750°C of Vanadium Steel [1]

<table>
<thead>
<tr>
<th>t, h</th>
<th>N \cdot 10^{-10} cm⁻³</th>
<th>\bar{r}, 10⁻⁵ cm</th>
<th>S_{\text{ext}}</th>
<th>r_{m}, 10⁻⁵ cm</th>
<th>r_{m}', 10⁻⁵ cm</th>
<th>r_{x}, 10⁻⁵ cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>111.79</td>
<td>2.45</td>
<td>1.39</td>
<td>2.486</td>
<td>2.57</td>
<td>2.59</td>
</tr>
<tr>
<td>30</td>
<td>22.99</td>
<td>2.98</td>
<td>1.96</td>
<td>3.513</td>
<td>1.71</td>
<td>1.97</td>
</tr>
<tr>
<td>50</td>
<td>17.73</td>
<td>3.72</td>
<td>2.06</td>
<td>3.984</td>
<td>2.57</td>
<td>2.44</td>
</tr>
<tr>
<td>75</td>
<td>12.16</td>
<td>3.54</td>
<td>2.44</td>
<td>6.129</td>
<td>2.10</td>
<td>1.93</td>
</tr>
<tr>
<td>100</td>
<td>16.58</td>
<td>2.96</td>
<td>3.20</td>
<td>11.158</td>
<td>1.71</td>
<td>1.22</td>
</tr>
</tbody>
</table>

(skewness) S_{k}, and the excess (kurtosis) ex. From the data in the table, it follows that: over the isothermal holding time of the steel at 750°C, a decrease occurs in the total number of microparticles; \bar{r} increases, reaches a maximum, and then decreases; the maximum of the distributions regularly shifts toward smaller sizes, which corresponds to a change over time in \( r_{m} \) and the asymmetry coefficient S_{k}; the excess of the distributions ex changes appreciably over time. But which internal processes in the steel cause such a change in the characteristics of the distributions? The data in Table 1 do not answer this question.

We need to establish a correlation between the indices of the transformation of the experimental histograms and the intrasystem processes causing it. With this goal, from the set of theoretical distribution functions in [2-4] we selected one similar to the experimental histogram with respect to congruence and we determined the corresponding parameters \( \alpha \) and \( \epsilon \). Using the computer program constructed, we examined the solution of the system of functionals \( S_{1}, S_{2} \) (see relation (4) in [2]) and the additional functional

\[
S_{3} = -2\epsilon_{v_{cr}} \sigma^{5}(1 + \alpha) r_{cr}^{-2\epsilon+4} M_{5+2\epsilon} - 2\epsilon \sigma_{v_{cr}}(1 + \alpha) r_{cr}^{-3} M_{4+\alpha} + 3r_{cr}^{-1} M_{2+\alpha} +
\]

\[
+ \sigma (5 + 2\alpha) r_{cr}^{-2\epsilon} M_{3+2\epsilon} - \epsilon (5 + 2\alpha) r_{cr}^{-1} M_{2+\alpha} - 3M_{1+\alpha} = 0
\]

for the condition of their minimization \( f = |S_{1}| + |S_{2}| + |S_{3}| = \min \) and maximum agreement between the modal radii \( r_{m} \) and \( r_{m}' \) of the distributions.*

The data for the sample calculation are shown in Table 2. The experimental maximum of the histogram corresponds to the size \( r_{m} = 2.57 \cdot 10^{-5} \) cm, and the maximum of the similar theoretical distribution is at \( \alpha = 0.307 \) and \( \epsilon = 0.02 - r_{m}' = 2.59 \cdot 10^{-5} \) cm. However, we should note that the numerical value of the experimental modal radius \( r_{m} \) is found within the limits of a single step of the division of the entire interval of the microparticle sizes.

Then, if a few very large microparticles occur in the dispersed system, the probability of their intersecting the plane of the metallographic section at a great circle is practically equal to zero. This indeterminacy in the calculations was eliminated by variation of the upper size limit \( r_{g}' \) within the limits of allowable values, for the condition that the quantity \( f \) attains a minimum. For this reason, the experimental values of \( r_{g} \) and the calculated \( r_{g}' \) (Table 1) may not coincide. The values of the moments of the distributions about \( r = 0 \) presented in Table 2 and included in the set of functionals \( S_{1}, S_{2}, \) and \( S_{3} \) contain some information on the change in shape of the curve for the microparticle size distribution. The comparison should be made between the integral moment and the fractional moments corresponding to it, for example \( M_{2} \) with \( M_{2,\alpha} \) and \( M_{2+\alpha} \). This mathematical problem requires an independent investigation.

Let us introduce additional parameters: the second and third moments of the distribution about the modal \( r_{m} \) and the critical \( r_{cr} \) radii of the microparticles and the corresponding internal asymmetry coefficients \( S_{k}(m) \) and \( S_{k}(cr) \). Let us do this in analogy with the external \( S_{k} = m_{3} / \sigma_{3}^{3/2} \), where the quantity \( \sigma = \int_{0}^{\bar{r}} (\bar{r} - r)^{2} \phi(r, t) dr \) and \( m_{3} = \int_{0}^{\bar{r}} (\bar{r} - r)^{3} \phi(r, t) dr \), substituting instead of \( \bar{r} \) the radii \( r_{m} \) and \( r_{cr} \) respectively. For known \( \alpha \) and \( \epsilon \), the values of the quantities \( u_{g} = r_{g}^{2} / r_{cr} \) \( r_{cr} \) \( c_{v} \) (the reduced velocity of motion of \( r_{cr} \) in the ensemble of sizes) and \( u_{m} = r_{m} / r_{cr} \) can be determined using formulas (1)-(3) in [2].

*Done jointly with A. F. Kulikov.