The compound-like nanosegregation at dislocations and grain boundaries in metallic materials, relevance to physics of the diffusion anomalies

Yury S. Nechaev

I.P. Bardin Central Research Institute for Ferrous Metallurgy, G.V. Kurdyumov Institute of Metals Science & Physics, Moscow, Russia
yuri1939@inbox.ru

According to [1-9], **the apparent diffusion coefficient of an impurity** (**D_Σ**) in metallic systems with dislocations (⊥s) or grain boundaries (GBs), **for the regime A,** can be described as:

$$D_\Sigma = [D\cdot(1-\eta_{\perp GB}) + D_{\perp GB}\cdot\eta_{\perp GB}(\partial C_{\perp GB}/\partial C)] \,/\, [1-\eta_{\perp GB} + \eta_{\perp GB}\cdot(\partial C_{\perp GB}/\partial C)], \qquad (1)$$

$$C_\Sigma \approx C\cdot(1-\eta_{\perp GB}+\eta_{\perp GB}\cdot K_{\perp GB}),\;\; K_{\perp GB} \approx (\partial C_{\perp GB}/\partial C) \approx (C_{\perp GB}/C) \approx exp(\Delta S_B/R)\cdot exp(-\Delta H_B/RT), \qquad (2, 3)$$

$$\boldsymbol{D_{\perp GB} \approx (D_\Sigma\cdot C_\Sigma - D\cdot C) \,/\, (C_\Sigma - C)}, \qquad (4)$$

where ΔH_B (< 0) is the bonding energy with ⊥s or GBs; $D_{\perp GB}$ is the diffusion coefficient in ⊥s or GBs.
If ($\eta_{\perp GB}\cdot K_{\perp GB}$) <<1, then $\boldsymbol{D_\Sigma \approx [D + D_{\perp GB}\cdot\eta_{\perp GB}\cdot K_{\perp GB}]}$ – the Hart-Mortlock type equation ($\boldsymbol{D_\Sigma > D}$); it is the case of the Cottrell type nanosegregation, which can be "easy diffusion paths".
If ($\eta_{\perp GB}\cdot K_{\perp GB}$) >>1, then $\boldsymbol{D_\Sigma \approx [D_{\perp GB} + (D/\eta_{\perp GB}\cdot K_{\perp GB})]}$ – the modified Oriani type equation ($\boldsymbol{D_\Sigma < D}$); it is the case of the non-Cottrell (compound-like) nanosegregation, it can be non-easy diffusion paths.

Some systems and diffusion processes are in detail considered [1-9], including the following ones: (1) the hydride-like nanosegregation of hydrogen at dislocations and grain boundaries in palladium and their influence on the apparent characteristics of hydrogen solubility and diffusivity in palladium; (2) the physics of the anomalous characteristics of diffusion of Fe and other transition impurities in crystalline Al at elevated temperatures, the role of the compound-like nanosegregation (CLNS) of Fe and the others at dislocations and grain boundaries in Al, analysis of the Mössbauer and diffusion data on CLNS of Fe at grain boundaries and dislocations in Al; (3) some new physical aspects of internal oxidation and nitridation of metals (for Cu-0.3% Fe alloy/Cu_2O surface layer, and for (Ni-5% Cr) alloy / N_2 gas), the role of CLNS at dislocations and grain boundaries, study results on the large deviations from the classical theories predictions and their interpretation.

The possibility is considered of nanotechnology applications of the study results for creation of nanostructured metals with CLNS structures at grain boundaries, in order to obtain specific physical and mechanical properties of such cellural-type nanocomposites. In particular, it can be created complex hydride-like, carbide-like, carbohidride-like, nitride-like, carbonitride-like, boride-like, oxide-like or intermetallide-like nanosegregation structures at grain boundaries in such materials.

References

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