Short Range Order and Static Displacements of Atoms in Polycrystalline Solid Solution of Fe-5 at. %Re

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INTRODUCTION

Intensity of X-ray diffuse scattering depends on scattering vector **q** according expression [1]:

$I_D(\mathbf{q})=nc_Ac_B\Sigma_jC_j\alpha_j\langle[<f>\mathbf{qA}(\mathbf{q})-(f_A-f_B)]^2\exp(i\mathbf{qR}_j)\rangle_{\varphi,\gamma}$, (1)

where n is number of atoms in primitive shell, c_A and c_B are concentrations of components, C_j is number of atoms on j- th shell, $\mathbf{R}_j$ is radii of j –th shell, α_j is short range order parameter on j – th shell, $\langle\ldots\rangle_{\varphi,\gamma}$ means averaging by all orientation of **q**, f_A and f_B are scattering form factors of atoms, $<f>=c_Af_A+c_Bf_B$, $\mathbf{A}(\mathbf{q})$ is vector parameter, which enters to expression for Fourier transform of static displacement $\delta\mathbf{R}_s$ of atom on s –th point of lattice:

$$\delta\mathbf{R}_s = i\sum_{\mathbf{q}}\mathbf{A}(\mathbf{q})c_{\mathbf{q}}\exp(-i\mathbf{qR}_s)\,;$$

$$c_{\mathbf{q}} = \frac{1}{N}\sum_{s=1}^{N}(c_s-c)\exp(i\mathbf{qR}_s), \qquad (2)$$

where c_s is occupation number on s –th point of lattice, c is concentration of alloy. It is possible to calculate the components of A(**q**) from following equations

$$D_{m\tau}(\mathbf{q})\,A_\tau(\mathbf{q}) = -iF_m(\mathbf{q}), \qquad (3)$$

where $D_{m\tau}(\mathbf{q})$ are elements of dynamical matrix expressed in [3] by force constants of interatomic interaction: $\varepsilon_j=\left(\frac{d^2V}{dR^2}\right)_{R_j}$; $\beta_j=\left(\frac{dV}{RdR}\right)_{R_j}$, where V(R) is pairwise interatomic potential, $F_m(\mathbf{q})$ is Fourier transform of m-th component of quasi restoring forces, which we developed in frame of De Launay model [2] in following form

$F_m=i\sigma_1(8/3)\sin(aq_m/2)\cos(aq_{m+1}/2)\cos(aq_{m+2}/2)+$
$+2i\sigma_2\sin(aq_m)+$
$2i\sigma_3\sin(aq_m)\{\cos(aq_{m+1})+\cos(aq_{m+2})\}$
$+i\sigma_4[(72/11)\sin(3aq_m/2)\cos(aq_{m+1}/2)\cos(aq_{m+2}/2)+$
$+(8/11)\sin(aq_m/2)\{\cos(3aq_{m+1}/2)\cos(aq_{m+2}/2)+$
$+\cos(aq_{m+1}/2)\cos(3aq_{m+2}/2)\}]+$
$+i\sigma_5(8/3)\sin(aq_m)\cos(aq_{m+1})\cos(aq_{m+2})+$
$2i\sigma_6\sin(aq_m)+$
$+i\sigma_7[(8/19)\sin(aq_m/2)\cos(3aq_{m+1}/2)\cos(3aq_{m+2}/2)+$
$+(72/19)\sin(3aq_m/2)\{\cos(3aq_{m+1}/2)\cos(aq_{m+2}/2)+$
$+\cos(aq_{m+1}/2)\cos(3aq_{m+2}/2)\}]++$
$+i\sigma_8[(16/5)\sin(2aq_m)\{\cos(aq_{m+1})+\cos(aq_{m+2})\}+$
$+(4/5)\sin(aq_m)\{\cos(2aq_{m+1})+\cos(2aq_{m+2})\}+$
$+i\sigma_9[(16/3)\sin(2aq_m)\cos(2aq_{m+1})\cos(2aq_{m+2})+$
$+(4/3)\sin(aq_m)\{\cos(2aq_{m+1})\cos(aq_{m+2})+$
$+\cos(aq_{m+1})\cos(2aq_{m+2})\}]$. (4)

(m=1,2,3; 1↔x, 2↔y, 3↔z).

RESULTS

The parameter α_j ,β_j and σ_j of pairwise interatomic inreaction of Fe-5 at. %Re were calculated by pseudopotential method [4]. Intensity of of X-ray diffuse scattering on Fe-5 at. %Re was measured in our early work [5].

By using suggested microscopic method for accounting of static displacements we defined from experimental intensity of X-ray diffuse scattering the short range order parameters of Fe-5 at. %Re alloy on nine shells: α_1=-0.038; α_2= 0.053; α_3=0.022; α_4=-0.034; α_5=0.049; α_6=0.103; α_7=-0.026; α_8=0.027; α_9= -0.020.

Meanwhile, in [5] via macroscopic method for accounting of static displacements were determined short range order parameters on four shells of Fe-5 at.%Re : α_1=-0.022; α_2= 0.028; α_3=-0.005; α_4=0.008.

CONCLUSION

Due to application of microscopic method for accounting of static displacements of atoms it is possible to determinate short range order parameters in binary alloy with body centered cubic structure on first nine shells.

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