Russian Physics Journal, Vol. 56, No. 6, November, 2013 (Russian Original No. 6, June, 2013)

DYNAMIC MODEL OF THE $B2 \rightarrow B19'$ MARTENSITIC TRANSFORMATIONS TAKING INTO ACCOUNT AN INTERMEDIATE MESOSCOPIC STATE

M. P. Kashchenko[1,2] **and V. G. Chashchina**[1,2]

UDC 669.018.2

It is demonstrated that the notion of the intermediate mesoscopic state during the $B2 \rightarrow B19'$ *transformation is constructive for a description of the observed morphological parameters. The* $\{78\ 39\ 48\}_{B2}$ *habit planes of the B19′ phase can be associated with standard dislocation nucleation centers. The results obtained are briefly discussed.*

Keywords: dynamic model, martensitic transformation, intermediate mesoscopic state, morphological parameters.

INTRODUCTION

As indicated in [1], the $B19'$ phase can be formed directly from the $B2$ phase after (or simultaneously with) the $B2$–$B19$ and $B2$–R transitions. In particular, the possibilities for initiation of the direct $B2$–$B19(19')$ transformation with the formation of the habit planes close to $\{78\,39\,48\}_{B2}$ observed in [2] within the limits of the concepts of heterogeneous nucleation and wave growth were studied in [3–6]. Based on the data about the orientational relationships between the lattice of Ti_3Ni_4 particles (precipitated in the process of aging) and the lattice of the $B2$ phase, the dislocation with line orientation $<1\,\bar{2}\,0>_{B2}$ associated with the elastic field of particles and untypical for the homogeneous $B2$ phase was chosen. It was demonstrated that this dislocation can play the role of a nucleation center for crystals with habit planes $\{78\,39\,48\}_{B2}$ and for crystals with habit planes $\{0.868\ 0.269\ 0.414\}_{B2}$ observed in [7]. The present work is aimed at demonstration of the fact that the $\{78\,39\,48\}_{B2}$ habit planes for crystals of the $B19'$ phase can also be associated with standard orientations of dislocation lines $\Lambda \parallel <111>_{B2}$ and $\Lambda \parallel <110>_{B2}$. For this purpose, it must be taken into account that the initial stage of forming the $B19'$ phase is associated with the influence of elastic fields of dislocations inherited by an intermediate mesoscopic state (IMS) after the $B2 \rightarrow$ IMS transition.

1. ORIENTATION OF DISLOCATION LINES OF NUCLEATION CENTERS DURING THE $B2 \rightarrow$ IMS $\rightarrow$ $B19'$ TRANSFORMATIONS

It is considered that the IMS arises due to fast strain of the $(01\bar{1})_{B2}$ plane initiated by the control wave process (CWP). The IMS variant arising after compression strain $\varepsilon_2 = (a_{B19} - a_{B2})/a_{B2} \approx -0.04917$ along the $[100]_{B2}$ direction and tensile strain $\varepsilon_1 = (c'_{B19} - \sqrt{2}\,a_{B2})/(\sqrt{2}\,a_{B2}) \approx 0.05343$ along the $[011]_{B2}$ direction is discussed here. The IMS $\rightarrow B19$ transition is accompanied by additional tension in the $[011]_{B2}$ direction (and small strain in the $[01\bar{1}]_{B2}$ direction that can be neglected in the first approximation). The IMS $\rightarrow B19'$ transition is accompanied by additional tension along the $[011]_{B2}$ direction and compression along the $[01\bar{1}]_{B2}$ direction. Additional interest in an analysis of variants of the

---

[1]Ural Federal University Named after the First President of Russia B. N. El'tsin, Ekaterinburg, Russia; [2]Ural State Forest Engineering University, Ekaterinburg, Russia, e-mail: mpk46@mail.ru. Translated from Izvestiya Vysshikh Uchebnykh Zavedenii, Fizika, No. 6, pp. 39–43, June, 2013. Original article submitted April 10, 2013.

$B2 \rightarrow B19'$ rearrangement with participation of intermediate phases is dictated by the possibility for obtaining arguments in support (though indirect) of material orientational relationships (OR) of the form

$$(011)_{B2} \,\|\, (001)_{B19}, \tag{1}$$

$$\varphi(æ) = \arccos \frac{\Gamma + æ^2}{\sqrt{(\Gamma^2 + æ^2)\,(æ^2 + 1)}}, \; \Gamma = \frac{1+\varepsilon_1}{1-|\varepsilon_2|}. \tag{2}$$

In Eq. (2), the angle $\varphi(æ)$ assigns misorientation of the corresponding directions, and the parameter æ is expressed by the relationship

$$æ = \frac{v_2}{v_1} = k \approx \sqrt{\frac{\varepsilon_1}{|\varepsilon_2|}}, \tag{3}$$

where v_1 and v_2 are moduli of the velocities of waves in the CWP. The introduction of the material OR is discussed in detail in [8, 9]. We note that in the particular case $\varphi(æ) = 0$, Eqs. (1) and (2) in the process of the $B2 \rightarrow B19$ transformation in single crystals are reduced to the Bain equations:

$$(011)_{B2} \,\|\, (001)_{B19},\; [100]_{B2} \,\|\, [100]_{B19},\; [01\bar{1}]_{B2} \,\|\, [010]_{B19}. \tag{4}$$

We believe that rearrangement of unit cells during the $B2$–IMS transition in the basis of the $B2$ phase is assigned by strains

$$\varepsilon_{[01\bar{1}]} \approx 0,\; \varepsilon_{[011]} \approx 0.04362,\; \varepsilon_{[100]} \approx -0.04917, \tag{5}$$

and the ratio $\varepsilon_{[011]} / |\varepsilon_{[100]}|$ can be matched with that of the wave velocities given by equalities (3). The transition to the basis $[01\bar{1}]_{B2}$, $[011]_{B2}$, and $[100]_{B2}$ from the $<100>_{B2}$ axes is performed by rotation around the $[100]_{B2}$ direction through the angle $\pi/4$.

As probable dislocation nucleation centers (DNC), we consider dislocations with lines $\mathbf{\Lambda}$ along the symmetry axes (of the second and third orders, respectively). We consider that these DNC are inherited by the IMS thereby changing the orientation of lines $\mathbf{\Lambda}$ by $\mathbf{\Lambda}'$ due to strain of unit cells and of lines $\mathbf{\Lambda}'$ by $\mathbf{\Lambda}''$ due to material rotation (2). In spite of the fact that the rotation angle is $\varphi(æ) \approx 2.6516^\circ$, we hope that some of the Λ'' lines will be in the habit planes of single crystals (or, taking into account experimental errors, will form the least angles with the habit planes). Preference for the DNC potential capable of initiating the wave variant of control over the crystal growth should be given exactly to the dislocations with such lines. We now check the above assumption by calculating the spectrum of directions $\mathbf{\Lambda}''$.

After strain (5), returning to the initial basis $<100>_{B2}$, we have

$$\begin{gathered}
[110]_{B2} \rightarrow [(1 + \varepsilon_{[100]}),\, 0.5(2 + \varepsilon_{[011]}),\, 0.5(\varepsilon_{[011]})]_{B2}, \\
[1\bar{1}0]_{B2} \rightarrow [(1 + \varepsilon_{[100]}),\, -0.5(2 + \varepsilon_{[011]}),\, -0.5(\varepsilon_{[011]})]_{B2}, \\
[101]_{B2} \rightarrow [(1 + \varepsilon_{[100]}),\, 0.5(\varepsilon_{[011]}),\, 0.5(2 + \varepsilon_{[011]})]_{B2}, \\
[\bar{1}01]_{B2} \rightarrow [-(1 + \varepsilon_{[100]}),\, 0.5(\varepsilon_{[011]}),\, 0.5(2 + \varepsilon_{[011]})]_{B2}, \qquad (6) \\
[011]_{B2} \rightarrow [0,\, (1 + \varepsilon_{[011]}),\, (1 + \varepsilon_{[011]})]_{B2}, \\
[01\bar{1}]_{B2} \rightarrow [01\bar{1}]_{B2},
\end{gathered}$$

$$[111]_{B2} \rightarrow [(1+ \varepsilon_{[100]}), (1 + \varepsilon_{[011]}), (1+ \varepsilon_{[011]})]_{B2},$$

$$[1\bar{1}1]_{B2} \rightarrow [(1 + \varepsilon_{[100]}), \bar{1}, 1]_{B2},$$

$$[11\bar{1}]_{B2} \rightarrow [(1 + \varepsilon_{[100]}), 1, \bar{1}]_{B2},$$

$$[\bar{1}11]_{B2} \rightarrow [-(1 + \varepsilon_{[100]}), (1 + \varepsilon_{[011]}), (1 + \varepsilon_{[011]})]_{B2}.$$

Directions (6) correspond to images Λ' of the symmetry axes of the second and third orders after strain (5), that is, when the Bain-type OR

$$[011]_{B2} \| [001]_{B19'}, [100]_{B2} \| [100]_{B19'}, (01\bar{1})_{B2} \| (010)_{B19'} \tag{7}$$

are satisfied. Though no one of the directions $\mathbf{\Lambda}$ or $\mathbf{\Lambda}'$, described by Eqs. (6), lies in the $\{78\ \ 39\ \ 48\}_{B2}$ planes, any line $\mathbf{\Lambda}'$ can be matched with the habit planes that form angles θ with it smaller than the angle θ between the initial line $\mathbf{\Lambda}$ and the same habit plane.

Similarly, during the $\mathbf{\Lambda}' \rightarrow \mathbf{\Lambda}''$ transformation associated with the lattice rotation, only one of the two rotation directions further decreases to θ the angle between $\mathbf{\Lambda}''$ and the habit plane. In Table 1, the data exactly for these orientations are given. Signs plus or minus in the second column $\mathbf{\Lambda}$ specify the directions of material rotation (2) through angles $\varphi(æ) \approx \pm 2.6516^{\circ}$ about the $[01\bar{1}]_{B2}$ axis. According to the data presented in Table 1, the least angles are $\theta'' \approx 0.15^{\circ}$ for $\mathbf{\Lambda}''$ associated with the pair of orientations $\mathbf{\Lambda}$ from the $<111>_{B2}$ family.

There are also small angles equal to 0.48° between $\mathbf{\Lambda}''$ associated with the $<110>_{B2}$ lines and the $\{78\ 39\ 48\}_{B2}$ planes. We note that double degeneration (not included in Table 1) of orientations of the matched $\mathbf{\Lambda}''$ habit planes that can differ by the least and average indices 0.39 and 0.48 is observed. The variants for θ'' that do not exceed 1° are also presented in Table 1. This implies that dislocations with lines $\mathbf{\Lambda}''$ associated not only with the initial directions $\mathbf{\Lambda} \| <110>_{B2}$ but also with the directions $\mathbf{\Lambda} \| <111>_{B2}$ of the lines inherited by the DNC during the $B2 \rightarrow \text{IMS} \rightarrow B19'$ rearrangement can be considered as potential nucleation centers.

Thus, there are grounds to consider that the martensite crystals with the $\{0.78\ 0.39\ 0.48\}_{B2}$ habit planes are associated with nucleation in elastic fields of dislocations with lines whose orientations practically coincide with the habit planes after strain (5) and material rotation (2). This indirectly confirms the correctness of OR (1) and (2).

2. DIRECTIONS OF WAVE NORMALS IN THE CWP STRUCTURE THAT ASSIGN THE HABIT PLANES OF THE CRYSTAL

Since the elastic anisotropy in titanium nickelide alloys near the transition point is usually small, it is convenient for the simplicity and vivid presentation to take advantage of the approximation of an isotropic medium. Then to find the pair of wave normals $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$ for wave beams in the CWP structure, the following procedure is necessary. In the beginning, it is necessary to calculate the vector product of $\mathbf{\Lambda}''$ and of the normal $\boldsymbol{N}_{\mathrm{w}}$ to the habit plane to find the line $\tilde{\boldsymbol{l}}$ of intersection of planes orthogonal to $\mathbf{\Lambda}''$ and $\boldsymbol{N}_{\mathrm{w}}$. Then we find the wave normals by rotating the intersection line through angles ±π/4 about $\mathbf{\Lambda}''$, which is equivalent to the relationships

$$\boldsymbol{n}_1 + \boldsymbol{n}_2 = \sqrt{2}\, \tilde{\boldsymbol{l}}/\tilde{l},\ \boldsymbol{n}_2 - \boldsymbol{n}_1 = \sqrt{2}\, \boldsymbol{N}_{\mathrm{w}}/N_{\mathrm{w}}, \tag{8}$$

from which we obtain

$$\boldsymbol{n}_1 = (\tilde{\boldsymbol{l}}/\tilde{l} - \boldsymbol{N}_{\mathrm{w}}/N_{w})/\sqrt{2}\,,\ \boldsymbol{n}_2 = (\tilde{\boldsymbol{l}}/\tilde{l} + \boldsymbol{N}_{\mathrm{w}}/N_{\mathrm{w}})/\sqrt{2}\,. \tag{9}$$

From Table 1 it follows that for the DNC associated with the initial directions $\mathbf{\Lambda} \| <110>_{B2}$, the wave normals in the approximation of small integer indices are close to $<\bar{1}10>_{B2}$ and $<001>_{B2}$. For the DNC associated with the initial

TABLE 1. Transformation of Orientations of Dislocation Lines **Λ** during the $B2 \rightarrow$ IMS Conversion (Strain (5) and Rotation through Angles φ(æ) ≈ ± 2.6516° about the $[01\bar{1}]_{B2}$ Axis)

N_w	Λ	Λ′	Λ″	θ′, °	θ″, °	n_1	n_2
0.48	$[1\bar{1}0]$ +	0.95083	0.915672	1.69	0.48	0.748286	0.066354
0.39		–1.02181	–1.052355			0.653281	0.099211
0.78		–0.02181	–0.052355			0.115289	–0.992852
–0.48	$[101]$ –	0.95083	0.983952	1.69	0.48	0.748286	0.066354
0.78		0.02181	–0.009853			–0.115289	0.992852
0.39		1.02181	0.990147			–0.653281	–0.099211
0.48	$[\bar{1}01]$ +	–0.95083	–0.915672	1.69	0.48	0.748286	0.066354
0.78		0.02181	0.052355			0.115289	–0.992852
0.39		1.02181	1.052355			0.653281	0.099211
0.48	$[110]$ –	0.95083	0.915672	1.69	0.48	0.748286	0.066354
–0.39		1.02181	1.052355			–0.653281	–0.099211
–0.78		0.02181	0.052355			–0.115289	0.992852
0.48	$[\bar{1}11]$ +	–0.95083	–0.881533	1.62	0.15	–0.167264	–0.849197
–0.39		1.04362	1.0736067			–0.763743	–0.209673
0.78		1.04362	1.0736067			0.623473	–0.484667
0.39	$[\bar{1}11]$ +	–0.95083	–0.881533	1.89	0.71	–0.271086	–0.849197
–0.48		1.04362	1.0736067			–0.789231	–0.209673
0.78		1.04362	1.0736067			0.552275	–0.484667
–0.48	$[111]$ –	0.95083	0.881533	1.62	0.15	–0.167264	–0.849197
–0.39		1.04362	1.073607			0.763743	0.209673
0.78		1.04362	1.073607			–0.623473	0.484667
–0.39	$[111]$ –	0.95083	0.881533	1.89	0.71	–0.271086	–0.825156
–0.48		1.04362	1.073607			0.789231	0.107298
0.78		1.04362	1.073607			–0.552275	0.555865
0.48	$[1\bar{1}1]$ +	0.95083	0.949812	2.24	1	0.141749	0.823682
0.78		–1	1.031104			0.593527	–0.514613
0.39		1	–0.968896			0.792233	0.238163
–0.48	$[1\bar{1}1]$ –	0.95083	0.949812	2.24	1	0.141749	0.823682
0.39		–1	–0.968896			0.792233	0.238163
0.78		1	1.031104			0.593527	–0.514613
0.48	$[11\bar{1}]$ +	0.95083	0.949812	2.24	1	–0.141749	–0.823682
0.39		1	1.031104			0.792233	0.238163
0.78		–1	–0.968896			0.593527	–0.514613
–0.48	$[11\bar{1}]$ –	0.95083	0.949812	2.24	1	–0.141749	–0.823682
0.78		1	–0.968896			–0.593527	0.514613
0.39		–1	1.031104			–0.792233	–0.238163

directions $\mathbf{\Lambda} \parallel \langle\bar{1}\,11\rangle_{B2}$, the wave normals are close to $\langle\bar{1}\,\bar{5}\,4\rangle_{B2}$, $\langle 3.7\ \ 1\ \ 2.2\rangle_{B2}$ and $\langle\bar{1}\,\bar{5}\,4\rangle_{B2}$, $\langle 4\ \ 1\ \ 2.2\rangle_{B2}$. It is easy to be convinced that in the approximation of the isotropic medium, the DNC with the line $\mathbf{\Lambda} \parallel [111]_{B2}$ can initiate growth of the martensite crystal with the $(11\bar{2})_{B2}$ habit plane and wave normals $\boldsymbol{n}_{1,2} \parallel \left[1 \pm \sqrt{3}\ \ 1 \mp \sqrt{3}\ \ \bar{2}\right]_{B2}$ that in the approximation of small integer indices correspond to $\left[4\ \bar{1}\ \bar{3}\right]_{B2}$ and $\left[\bar{1}\ 4\ \bar{3}\right]_{B2}$. The $\mathbf{\Lambda} \rightarrow \mathbf{\Lambda}''$ transition is accompanied by deviations of the wave normals and the $(11\bar{2})_{B2} \rightarrow (0.48\ 0.39\ \overline{0.78})_{B2}$ change of the habit plane.

Analogously, for $\mathbf{\Lambda} \| <\bar{1}10>_{B2}$, the habit planes $\{223\}_{B2}$ are observed with wave normals close to $\boldsymbol{n}_1 \| <\bar{1}10>_{B2}$ and $\boldsymbol{n}_2 \| <001>_{B2}$. The $\mathbf{\Lambda} \rightarrow \mathbf{\Lambda}''$ transition is accompanied by deviations of the wave normals and the $(22\bar{3})_{B2} \rightarrow (0.48\ 0.39\ \overline{0.78})_{B2}$ change of the habit plane. Hence there are grounds to believe that during the $B2 \rightarrow \text{IMS} \rightarrow B19'$ transformations there are actual possibilities for dynamic control over the martensite crystal growth [10–13] started in elastic fields of dislocations genetically related to the $B2 \rightarrow$ IMS structural rearrangement.

CONCLUSIONS

Our analysis has demonstrated that during the $B2 \rightarrow \text{IMS} \rightarrow B19'$ MT, consideration of final deformations and orientational relationships has allowed us to explain the observed orientations of the habit planes of the $B19'$ phases by choosing dislocations with standard initial orientations of lines $\mathbf{\Lambda} \| <110>_{B2}$ and $\mathbf{\Lambda} \| <111>_{B2}$ as the main DNC. These lines change when they inherit dislocations during the $B2 \rightarrow B19'$ transition. Thus, the use of orientations $\mathbf{\Lambda} \| <1\bar{2}0>_{B2}$ is not obligatory though possible [3–6]. This result indirectly confirms the correctness of OR (1) and (2), which makes expedient precision measurements of the OR to establish reliably their difference from the Bain relationships. Of interest is analogous analysis of the $B2 \rightarrow B19 \rightarrow B19'$ MT in which the phase $B19$ will play the role of the intermediate state.

This work was supported in part by the Russian Foundation for Basic Research (project No. 11-08-96020).

REFERENCES

1. Titanium Nickelide Alloys with Shape Memory. Part I. Structure, Phase Transformations, and Properties [in Russian], Publishing House of the Ural Branch of the Russian Academy of Sciences, Ekaterinburg (2006).
2. S. Miyazaki, K. Otsuka, and C. M. Wayman, Acta Metall., **37**, No. 7, 1873–1884 (1989).
3. N. V. Aristova, I. V. Alexina, and M. P. Kashchenko, Fiz. Met. Metallogr., **77**, No. 1, 146–150 (1994).
4. I. V. Alexina, N. V. Aristova, and M. P. Kashchenko, in: Shape Memory, International Academic Publishers, Beijing, China (1994), pp. 65–69.
5. M. P. Kashchenko, I. V. Alexina, V. V. Letuchev, and A. V. Nefedov, Fiz. Met. Metallogr., **80**, No. 6, 10–15 (1995).
6. V. V. Letuchev, V. P. Vereshchagin, and M. P. Kashchenko, J. Phys. IV, Colloque C8, **5**, 151–156 (1995).
7. O. Matsumoto, S. Miyazaki, K. Otsuka, and H. Tamura, Acta Metall., **35**, No. 8, 2137–2144 (1987).
8. M. P. Kashchenko and V. G. Chashchina, Dynamic Model of Forming Twinned Martensite Crystals during the γ–α Transformation into Iron Alloys [in Russian], Publishing House of the Ural State Forest Engineering University, Ekaterinburg (2009).
9. M. P. Kashchenko and V. G. Chashchina, Dynamic Theory of the γ – α Martensitic Transformation in Iron-Based Alloys. Solving the Problem of the Formation of Twinned Martensite Crystals, LAMBERT Academic Publishing, Saarbrucken, Germany (2012).
10. M. P. Kashchenko and V. G. Chashchina, Phys.–Usp., **54**, No. 4, 331–349 (2011).
11. M. P. Kashchenko and V. G. Chashchina, Pis'ma Mater., **1**, 7–15 (2011).
12. M. P. Kashchenko and V. G. Chashchina, Mater. Sci. Forum, **738–739**, 3–9 (2013).
13. M. P. Kashchenko, Wave Model of Martensite Growth during the γ–α Transformation into Iron-Based Alloys [in Russian], 2nd Edition, Scientific and Publishing Center "Regular and Chaotic Dynamics," Izhevsk Institute of Computer Science, Moscow; Izhevsk (2010).