self-accommodation effects were investigated to help with resolving this issue.

4.2. Modelling the local variant selection

To tentatively account for the formation of highly intricate, plate-shaped groups of laths sharing the same Bain zone, a micromechanical model, together with a mean field homogenisation technique, was used. In this model, the formation of the groups was supposed to be accompanied by a shape strain. There are several ways to evaluate the shape strain, including surface relief measurement. In this study, surface relief was observed but not quantitatively measured. Thus, the shape strain was estimated by using the habit plane indices and a phenomenological theory of martensite crystallography (PTMC). Modelling was performed in two steps:

Step 1: Selection and use of a PTMC theory according to experimental results and calculation of the shape strain induced by the phase transformation, which is then considered as an "eigenstrain" in Step 2.

Step 2: Use of the micromechanical model to calculate the stored energy and equivalent stress in austenite induced by formation of two highly intricate sets of groups in a given austenite grain.

4.2.1. Calculation of the shape strain and crystallographic features associated with the 24 bainite variants

The habit planes in the vicinity of the $\{111\}_\gamma$ and $\{557\}_\gamma$ plane families cannot be accounted for by the PTMC theories involving a single lattice invariant shear (LIS) system [18,42]. Here, a PTMC theory involving two LIS systems was used, namely, the model developed by Ross and Crocker [43] and applied by Kelly [44] to $\{223\}_\gamma$ and $\{557\}_\gamma$ lath martensite in steels. In this theory, the ("macroscopic") shape strain is an invariant plane strain leaving the habit plane undistorted and unrotated. It is decomposed as follows:

$$\mathbf{F} = \mathbf{R} \cdot \mathbf{B} \cdot \mathbf{S_2} \cdot \mathbf{S_1}, \tag{1}$$

where **F** is the shape strain, **B** is the Bain strain induced by the homogeneous lattice transformation from face-centered cubic into body-centered tetragonal structures, and $\mathbf{S_1}$ and $\mathbf{S_2}$ are the LIS strains. Here, they correspond to slip, as no internal twinning was revealed by TEM in the bainite laths. The Bain strain only depends on the lattice parameters of the two phases and on the lattice correspondence, i.e., on the particular variant investigated. Following Kelly [44], the low-carbon bainite phase was assumed to be cubic, and the lattice correspondence was the same as the one considered in the early theory of Bowles and Mackenzie [45], leading to the following equations:

$${}_\alpha\mathbf{C}_\gamma = \begin{pmatrix} 1 & 0 & 1 \\ 1 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix} \tag{2}$$

is the lattice (Bain) correspondence expressed in the $\langle 001\rangle_\alpha$ bainite frame.

$$\mathbf{B} = \begin{pmatrix} \eta_1 & 0 & 0 \\ 0 & \eta_2 & 0 \\ 0 & 0 & \eta_1 \end{pmatrix} \tag{3}$$

is the Bain strain expressed in the $\langle 001\rangle_\gamma$ austenite frame.

The input data are as follows. Lattice parameters are 3.59 Å for austenite and 2.86 Å for bainite [46]. The slip systems were taken from [44] to lead to a $\{557\}_\gamma$ habit plane. For the variant under consideration, the shear plane and directions are $(11\bar{5})[1\bar{1}0]_\gamma$ corresponding to $(\bar{2}31)[11\bar{1}]_\alpha$ for $\mathbf{S_1}$, and $(311)[0\bar{1}1]_\gamma$ corresponding to $(211)[1\bar{1}\bar{1}]_\alpha$ for $\mathbf{S_2}$, respectively. The shear amplitudes of $\mathbf{S_1}$ and $\mathbf{S_2}$ are g_1 and g_2. Thus, the strain tensors can be expressed as follows, in the austenite frame:

$$\text{for } \mathbf{S_1} : \mathbf{S_1} = \mathbf{I} + \frac{g_1}{|\mathbf{d_1}| \cdot |\mathbf{p_1}|} \cdot \mathbf{d_1} \otimes \mathbf{p_1}, \text{ and}$$
$$\text{for } \mathbf{S_2} : \mathbf{S_2} = \mathbf{I} + \frac{g_2}{|\mathbf{d_2}| \cdot |\mathbf{p_2}|} \cdot \mathbf{d_2} \otimes \mathbf{p_2}, \tag{4}$$

where **I** is the second-order identity tensor and for $i = 1, 2, \mathbf{d}_i$ is the shear direction, $\mathbf{p}_i$ is the shear plane, and g_i is the amount of shear. Following [44], the value of g_2 was chosen such that a $\{557\}_\gamma$ habit plane was obtained whatever the value of g_1, i.e., $g_2 = 0.130$.

The calculation outputs for the reference variant are the amount g_1 of first LIS $\mathbf{S_1}$, shape strain direction **d**

Table 3
Results of the PTMC calculations (following [44]), expressed in the $\langle 001\rangle_\gamma$ frame

Amount of first lattice invariant shear, g_1	0.224
Amount of macroscopic strain, m	0.490
Indices of the shape strain direction, **d**	$\begin{pmatrix} 0.3138 \\ -0.8363 \\ 0.4496 \end{pmatrix}_\gamma$
Indices of the habit plane normal, **h**	$(0.5025 \quad 0.5025 \quad 0.7035)_\gamma$
Angle between close-packed planes $(111)_\gamma$ and $(101)_\alpha$	0.19°
Angle between close-packed directions $[1\bar{1}0]_\gamma$ and $[11\bar{1}]_\alpha$	2.94°
Orientation relationship (axis–angle pair) between γ and α	51.15° around $\begin{pmatrix} 0.4697 \\ -0.7862 \\ 0.4017 \end{pmatrix}_\gamma$