Table 5
Results given by self-consistent modelling of accommodation between bainite variants

Pair of variants	Habit plane of second variant	Angle between habit planes	Misorientation angle	Stored elastic energy	Mean Von Mises equivalent stress in bainite (MPa)	Mean Von Mises equivalent stress in austenite (MPa)
1–1	$(5\,5\,7)_\gamma$	0°		1.00	392	392
1–2	$(\bar{7}\,\bar{5}\,\bar{5})_\gamma$	16.3°	4.7°	1.39	534	377
1–10	$(\bar{5}\,\bar{5}\,7)_\gamma$	89.4°	11.9°	1.72	654	321
1–23	$(\bar{5}\,\bar{5}\,\bar{7})_\gamma$	0°	60.3°	1.53	614	308

The value of stored energy is normalised by the value obtained for 50% of variant 1 alone.

The homogenisation method used a self-consistent scheme, although the underlying hypothesis of "perfect disorder" in the three-phase microstructure might not be fulfilled in the present case. Each of the three phases was in turn considered as an "Eshelby" inclusion embedded in an infinite matrix having the average ("homogenised") properties of the three-phase material [49]. Stress-free boundary conditions were applied to the infinite matrix. The elastic properties of the phases were assumed to be homogeneous and isotropic. Thus, coupling between phases only derives from the self-consistency assumption and from the disappearance of the mean stress tensor far from the inclusions.

Each inclusion I ($I = \gamma$ for austenite, $I = 1$ for variant 1, $I = N$ for the other variant, with $N = 1, 2, 10$, or 23) was attributed a fourth-order Eshelby tensor $\mathbf{S^I}$ (representing its geometry) and a second-order eigenstrain tensor $\boldsymbol{\varepsilon}^*_\mathbf{I}$. For bainite variants 1 and N, $\boldsymbol{\varepsilon}^*_\mathbf{I}$ is the transformation-induced shape strain determined in the previous section. The bainite variants were considered to remain elastic but plastic deformation was allowed in the austenite phase. Thus, $\boldsymbol{\varepsilon}^*_\gamma$ is the amount of plastic strain induced in austenite by the transformation of the two other phases. It was calculated using an iterative method by assuming an elastic–plastic constitutive behaviour for the austenite phase. The accuracy of values used for the coefficients does not affect the trends given by the model but affects the quantitative values, so that the following results can only be interpreted in a qualitative manner. Here, as a first step, the values were set as follows: Young's modulus $E = 2 \times 10^5$ Pa and Poisson ratio $\nu = 0.3$ for all phases, and for austenite, a yield strength of 300 MPa and an isotropic linear work-hardening rate of 5000 MPa. At each iteration step, the difference between the equivalent Von Mises stress in austenite and the yield stress given by the constitutive equation for the same equivalent plastic strain was calculated. If negative, the plastic strain amplitude was slightly increased along the normal to the Von Mises yield surface of the austenite phase. Convergence of results was reached as soon as the equivalent stress in the austenite phase was equal to the stress predicted using the constitutive equation and total equivalent strain in austenite. The total number of iterations was less than 100.

The equations used in the homogenisation model are as follows. The uniform stress in inclusion I is:

$$\sigma_\mathbf{I} = \mathbf{C} : (\mathbf{I} - \mathbf{S^I}) : (\mathbf{E}^* - \boldsymbol{\varepsilon}^*_\mathbf{I}), \quad \text{(Eshelby inclusion problem)} \tag{5}$$

where $\mathbf{C}$ is the fourth-order elasticity tensor, $\mathbf{I}$ is the fourth-order identity tensor and $\mathbf{E^*}$ is the average eigenstrain tensor, which is derived from the stress-free boundary conditions:

$$\left\langle \mathbf{I} - \mathbf{S^I} \right\rangle : \mathbf{E}^* = \left\langle (\mathbf{I} - \mathbf{S^I}) : \boldsymbol{\varepsilon}^*_\mathbf{I} \right\rangle, \tag{6}$$

where "$\langle\cdot\rangle$" denotes averaging over all three phases.

The calculations were carried out in the frame of the ellipsoid of variant 1. To solve the Eshelby problem, a small-scale deformation hypothesis had to be made, so that only the symmetric part of the shape strain matrices could be considered. Consistently with this, the shape strain amplitude was divided by ten, in order to satisfy the small-scale deformation assumption. This should not qualitatively affect the comparison between results obtained with the various pairs of variants.

4.2.3. Results given by the model

The stored energy (normalised by the value obtained with variant 1 alone i.e., $N = 1$) is given in Table 5 together with the Von Mises equivalent stress in the austenite phase. In terms of stored elastic energy, the most efficient accommodation is given by the single-variant configuration. This could explain why parallel groups of a given variant are frequently seen in micrographs (Fig. 3(a)). Nevertheless, this could also be at least partly due to the assumption of homogeneous and isotropic elastic properties of the material, while the micromechanical model handles with geometric and crystallographic features at the scale of the individual crystals. The mechanical behaviour of bainite also plays a significant role, as the major part of the elastic stored energy stems from the high stresses in the bainite inclusion. Allowing plastic deformation in bainite should significantly change the values of the energy stored in the system.

In terms of stress and plastic strain in the austenite phase, the single-variant configuration is clearly the less accommodating configuration. Variant 2, having the lowest misorientation with variant 1, does not allow