

Supplementary material 1:

Some crystallographical models of martensitic transformation.

1 Bain distortion

The history of martensitic transformation theories in steels or other Fe alloys can be traced backed when Bain (1924) proposed in his paper “The nature of martensite”, a simple distortion that allows a fcc lattice to be transformed into a bcc lattice. An intermediate tetragonal lattice is constructed from the fcc one by choosing the $\frac{1}{2} [110]_\gamma$, $\frac{1}{2} [\bar{1}10]_\gamma$ and $[001]_\gamma$ directions as new reference frame and by expanding the two first vectors by 12.6%, and reducing the third one by 20.3%, in order to obtain the bcc lattice with appropriate lattice parameters (Fig. S1_1). The Bain distortion is often reported to involve the smallest principal strains; however, to our knowledge Bain OR has been reported only in Fe-Pt alloys (Shimizu & Tanaka, 1978), and has never been observed in other martensitic iron alloys. Bain distortion is used in the Phenomenological Theory of Martensitic Transformation (PTMT) (see last section).

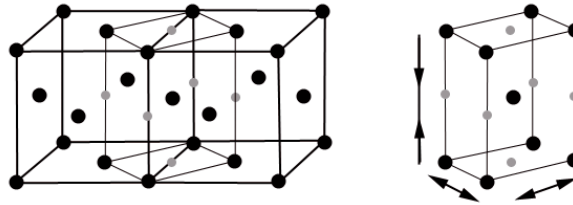


Fig. S1_1. Bain distortion (fcc-bct-bcc transformation). The Fe and C atoms are in black and grey, respectively. The distortion is a compression of 20% along the $[001]_\gamma$ axis and expansion of 12% along the $[110]_\gamma$ and $[\bar{1}10]_\gamma$ axes.

2 The KSN shear/distortive model

An alternative atomistic model, illustrated in Fig. S1_2, has been proposed later by Kurdjumov & Sachs (1930) and by Nishiyama (1934) in their original papers. In the 1930's, the dislocations were not yet discovered and the partial Shockley dislocations favouring the first step by an intermediate hcp ϵ phase could not be used as counter-argument to the critics

of Greninger & Troiano (1949) arguing that « *A more serious objection to these mechanisms is the relatively large movement and readjustments required* » (one can wonder why such objection was not also opposed to the Bain distortion at that time). The KSN model seems to have declined in the 1960's after the discovery by transmission electron microscopy (TEM) of twins in martensite. Their presence was “predicted” by the PTMT and was thus considered as the “*triumph*” of this theory (Kelly & Groves, 1973), even by Nishiyama if we consider that the KSN model takes less than one page and the PTMT a whole chapter in his book (Nishiyama, 1978). The KSN model is not anymore presented in modern books.

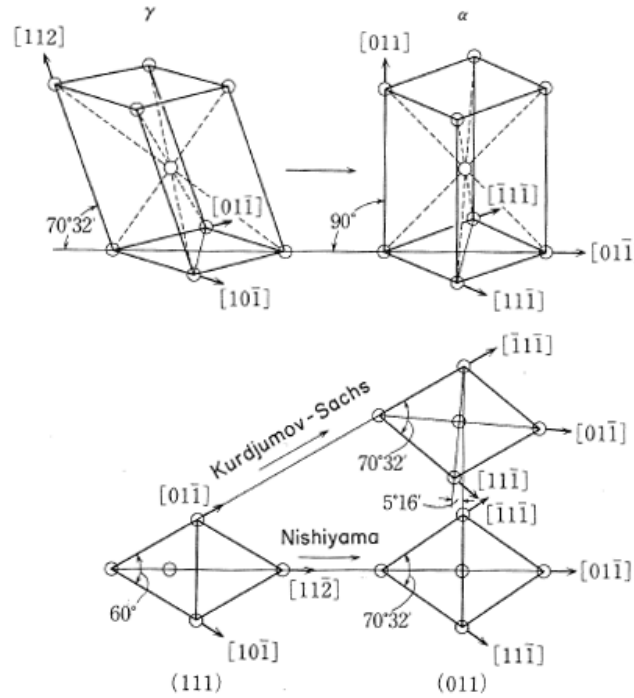
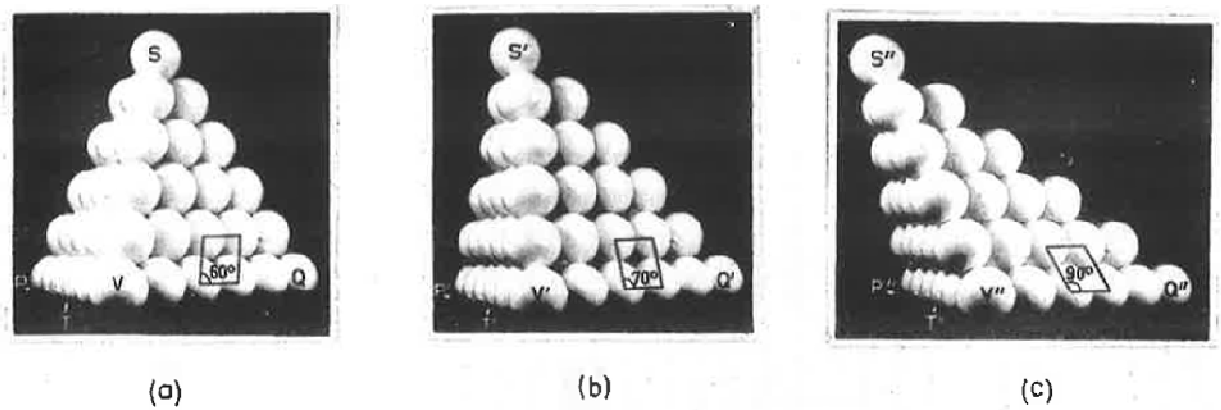


Fig. S1_2. KSN model of fcc-bcc transformation by a shear of 19.5° on the $(111)_\gamma$ plane on the $[11\bar{2}]_\alpha$ direction followed by a distortion of 10.5° (and shuffle). From Nishiyama book (1978).

3 The Bogers and Burgers model

Later, Bogers & Burgers (1964) developed an ingenious physical model based on hard sphere representation of the atoms (Fig. S1_3). They noticed that if a shear on a $(111)_\gamma$ plane is applied to a fcc crystal and stopped at a special position, the operation transforms the 60° angle in two other $\{111\}_\gamma$ planes (angle between the $\langle 110 \rangle_\gamma$ directions, Fig. S1_3a) into a 70.5° angle of the new $\{110\}_\alpha$ planes (angle between the $\langle 111 \rangle_\alpha$ directions, Fig. S1_3b). Another shear on another $(111)_\gamma$ plane is required to obtain the final bcc structure.



(a) Original tetrahedral arrangement with four $\{111\}$ planes.

(b) Intermediate position after $1/3$ of normal twin shear. The distance between successive $\{111\}$ planes parallel to $P'V'S'$ and $P'V'Q'$ has increased by 5.4% .

(c) Final position after complete twin shear.

Fig. S1_3. The Bogers and Burgers model. (a) Original packing of atoms in the fcc crystals, (b) after distortion by a shear on $\{111\}$ plane corresponding (b) to $1/3$ twin shear and (c) to a complete twin shear. From Bogers & Burgers (1964).

Their work was later refined by introducing Shockley partial dislocations, and promoted by Olson & Cohen (1972, 1976). It can be summarized as followed: the first shear is on a $\{111\}_\gamma$ plane of vector $1/8 \langle 112 \rangle_\gamma$, which can be achieved by $1/6 \langle 112 \rangle_\gamma$ Shockley partial dislocations averaging one over every second $(111)_\gamma$ slip plane, and the second shear is on another $\{111\}_\gamma$ plane of vector $1/18 \langle 112 \rangle_\gamma$, which can be achieved by $1/6 \langle 112 \rangle_\gamma$ Shockley partial dislocations averaging one over every third $(111)_\gamma$ slip plane. The former is noted $T/2$ and the latter $T/3$. This approach is in qualitative agreement with the observations of the martensite formation at the intersection of hcp plates or stacking faulted bands on two $(111)_\gamma$ planes. The model has an interesting physical base but its intrinsic asymmetry between the $\{111\}_\gamma$ planes with $T/2$ and $T/3$ seems to be too strict and ideal to be obtained in a real material.

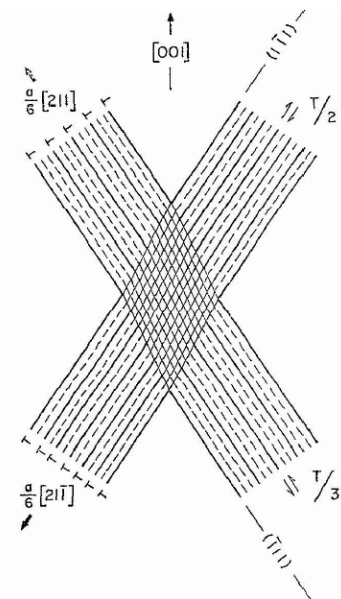


Fig. S1_4. The Olson-Cohen model. The α martensite is formed at the intersection of the two planar faults $T/2$ and $T/3$. From Olson & Cohen (1972).

The three models presented previously try to imagine the atomic movements of the iron atoms during the martensite transformation, but can't explain the shapes and habit plane of martensite. For example, as noticed by Greninger & Troiano (1949), the martensite transformation was supposed to result from a shear process, but the shear plane, assumed to be the habit plane, is not in agreement with neither the Bain distortion nor the experimentally observed ORs.

4 The phenomenological theory of martensite transformation (PTMT)

In order to reconcile the Bain distortion, the measured ORs and the HPs, the phenomenological theory of martensite transformation (PTMT), also called phenomenological theory of martensitic crystallography (PTMC), has been developed in the 1950's (Wechsler et al. 1953; Bowles & Mackenzie, 1954) and further promoted in many books (Kelly & Groves, 1973; Nishiyama, 1978; Bhadeshia, 1987; Christian, 2002). It takes the form of sequences of multiplications of matrices, each of them representing one part of the problem: a first simple shear P_1 (called invariant plane strain IPS) responsible for the macroscopic shape change and habit plane, and a second shear P_2 responsible for the structural change (without shape change). This last shear is the superposition of a classical homogeneous deformation and an inhomogeneous lattice invariant deformation produced by slip or twinning. The total transformation matrix $T = P_1 P_2$ is an invariant line deformation given by the intersection of the two shear planes. The theory assumes that this total transformation matrix can also be written as the initial Bain distortion B associated with a rigid body rotation R so that $T = BR$. The Bain distortion achieves the desired volume change between the γ and α crystals with the “*smallest*” strains. The PTMT was generalized and further complexified by incorporating multiple shear lattice invariant deformations (Acton & Bevis, 1969). PTMT is the most classical approach to martensite transformations and used in most of the studies that require strain/stress calculations. Other approaches based on strain energy considerations and interfacial dislocations models are also reported in the recent review of Zhang & Kelly (2009).