Martensite, a body centered cubic (BCC) derived metastable phase of iron and carbon, is the cornerstone of all hard steels. The martensite phase, often labeled the metastable phase of iron and carbon, is the cornerstone of the transformation and that this is a consequence of a plane that remains invariant during the transformation. Both of these models were based on the measured orientation relationships (OR) between the martensite grains and the residual austenite. The Kurdjumov-Sachs OR and Nishiyama-Wassermann OR, observed in carbon-iron and nickel-iron alloys, respectively, are the most commonly observed ORs. Other ORs have also been measured including the Greninger-Troiano OR and the Pitsch OR observed in thin films. In our own work, we start from the assumption that the most likely transformation mechanism is the one that requires the least displacement of all the atoms in the crystal. This is a plausible physical assumption that was employed by Jaswon and Wheeler in their paper that lead to the PTMT, in our previous work on phase transformations and in the works of others. Let us consider the cumulative distance $d_1$ traveled by $N$ atoms from austenite to martensite:

$$d_1 = \sum_{l=1}^{m} \sum_{i,j,k=-n}^{n} ||\mathbf{v}_{ijkl}^\gamma - \mathbf{v}_{ijkl}^\alpha||,$$

(1)

where $\mathbf{v}_{ijkl}$ are the position vectors of atoms of the initial austenite structure ($x = \alpha$) or the final martensite structure ($x = \gamma$) defined as:

$$\mathbf{v}_{ijkl}^x = C^x \left( \begin{array}{c} i \\ j \\ k \end{array} \right) + \mathbf{p}_l^x.$$

$C^x$ is a unit cell of either the martensite or the austenite, and $\{\mathbf{p}_l^x : l = 1 \ldots m\}$ are the atomic positions inside $C^x$. The total number of atoms in this bloc of material is $N = m(n-1)^3$. 

We present a unifying description for the martensitic transformation of steel that explains all of the important experimentally observed features. It is obtained through a geometric minimization of the total distance traveled by all the atoms from the austenite (FCC or $\gamma$) phase to the martensite (BCC or $\alpha$) phase. Our description unites previously proposed mechanisms but it does not rely on assumptions and experimental knowledge regarding the shear planes and directions, or external adjustable parameters. We show how the Kurdjumov-Sachs orientation relationship between the two phases and the $\{225\}_\gamma$ interfacial (habit) plane, which have both been extensively reported in experiments, naturally emerge from the distance minimization. We also propose an explanation for the occurrence of a different orientation relationship (Pitsch) in thin films.
The choice of the unit cell vectors (including their orientation in space) and the order in which the atoms are labeled (indexed) will determine the mechanism of the transformation. For example, in the Bain transformation, the FCC cell vectors ($C^\gamma$) would be $[110]a_\gamma/2$, $[\bar{1}0\bar{1}]a_\gamma/2$ and $[100]a_\gamma$, where $a_\gamma$ is the austenite lattice constant. The martensite cell vectors would be that of the conventional BCC cell rotated clockwise by 45° about the c-axis. There would be one atom at the origin and one at the center of both cells (the relative atomic positions would not change during the transformation). This particular choice of the $C^\gamma$ and $\{p^\gamma_l : l = 1...m\}$ for both structures fully describes the Bain transformation mechanism and it corresponds to a unique distance $d_1$.

Thus, the actual mechanism of transformation, according to our initial assumption, can be characterized by the set of $C^\alpha$ and $\{p^\alpha_l : l = 1...m\}$ that minimizes $d_1$ when $N \to \infty$. We have shown that the leading dependence of $d_1$ on the size ($N$) is a function of the distortion in the lattice, i.e., the strain. Therefore, by minimizing $d_1$, we also necessarily minimize the strain.

The Structure Matching Algorithm [24] we developed recently and applied to this problem is an iterative approach to minimizing $d_1$. It directly minimizes the distance travelled by all ($N$) atoms belonging to a section of the crystal that is chosen to be as large as possible (ideally $N \to \infty$). After minimizing $d_1$ our algorithm retrieves the periodicity or the scale of the transformation ($C^\alpha$) if it exists. We provide a brief explanation of how the algorithm works in the Supplementary Materials and a more detailed description of the method can be found in Ref. [24]. We wish to emphasize the fact that the algorithm requires only the initial and final structures as inputs and does not require adjusting any external parameters. We used our distance minimization algorithm to find the transformation of pure iron from FCC to BCC. For austenite, we used the lattice constant $a_\gamma = 3.585\,\text{Å}$. For martensite we use both the hard-sphere packing lattice constant [20] [25] ($a_\alpha = \sqrt{2/3}a_\gamma = 2.927\,\text{Å}$) and the experimentally measured lattice constant $a_\gamma = 2.87\,\text{Å}$ and applied our algorithm to both choices.

Fig. 1 shows the transformation mechanism that minimizes $d_1$ resulting from our structure matching algorithm. The optimal $C^\gamma$ and $C^\alpha$ with their atomic positions are illustrated in panel (a) and (b) respectively. From the $[110]_\gamma/[\bar{1}11]_\alpha$ perspective (blue frame in panel (c)) , going from FCC to BCC, one can see an elongation in the $[001]_\gamma/[\bar{1}0\bar{1}]_\alpha$ (green arrow) direction; it is particularly noticeable by looking at the change in shape of the FCC conventional cell in black. Now, looking in the $[001]_\alpha/[\bar{1}0\bar{1}]_\alpha$ direction (green frame), the transformation includes a shear of the $(1\bar{1}1)_\gamma/(1\bar{1}2)_\alpha$ plane in the $[110]_\gamma/[\bar{1}11]_\alpha$ direction with a slip every sixth layer. The initial and final cells are linked by a transformation matrix $T$ such that $TC^\gamma(\gamma) = C^\alpha(\gamma)$ called the deformation gradient matrix (the exponent in parenthesis indicates the basis). The matrix $T$ does not fully describe the transition because it does not account for the displacement of the atoms inside the cell. Indeed, from panel (a) to panel (b) in Fig. 1, not only the cells have been distorted, but the atoms inside them have been displaced. An animation of the transformation from the same viewing directions as in Fig. 1 and the evolution of the simulated X-ray diffraction patterns [26] along the transformation are provided in the supplementary material together with the crystal structures (POSCAR format) for 60 snapshots along the transformation for both possible orientation relationships (explained further in the text).

Let us first analyze the deformation gradient matrix $T$. According to the polar decomposition theorem, it can
always be written as $T = RU$ where $R$ is a rotation (unitary) matrix and $U$ is a symmetric matrix [27]. Consequently $U - I$ is a proper strain tensor and its eigenvalues are the principal strains of the transformation. One can show that the eigenvalues of $U$ are the square roots of the eigenvalues of $T^T T$ and their eigenvectors are the same. Our structure matching algorithm gives us the optimal $T$ directly, from which one gets:

$$U = P \begin{pmatrix} \frac{2\sqrt{2}}{3} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix} P^T, \quad P = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad (2)$$

where the columns of $P$ are the eigenvectors of $U$ in the basis of the FCC conventional cell. Similarly, in the basis of the BCC lattice going from BCC to FCC, the eigenvalues are inverse and the eigenvectors (columns of $P$) are given by:

$$Q = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & 0 \end{pmatrix} \quad (3)$$

Therefore, the principal strains $\lambda_i - 1$ are $-5.7\%$, $0\%$ and $15.5\%$. Those strains are significantly lower than the one resulting from the Bain, Pitsch, Nishiyama-Wassermann (N-W) and Kurdjumov-Sachs (K-S) deformation paths which are, using our lattice constants, $-18.4\%$, $15.5\%$ and $15.5\%$. The direction of the largest, $15.5\%$ strain in our solution is $[001]_\gamma/[[1\bar{T}0]_\alpha$ and therefore the two other principal strains lay in the plane perpendicular to it. In the Bain path, one of the two (degenerate) principal strains of $15.5\%$ can always be chosen to be in the same $[001]_\gamma/[[1T0]_\alpha$ direction. Therefore, the difference between our proposed mechanism and the Bain distortion lies entirely in the $(001)_\gamma/[[1T0]_\alpha$ plane. Using the experimental lattice parameter of 2.87Å for martensite, we obtain principal strains of $-7.2\%$, $1.6\%$ and $13.7\%$ compared with Bain strains of $19.7\%$, $13.7\%$, $13.7\%$ in that case. The strains are in the same crystallographic directions as for the hard-sphere packing lattice constant, i.e., $P$ and $Q$ do not change.

The reduction of strain in the $(001)_\gamma/[[1T0]_\alpha$ plane that we get is due to slipping and naturally emerges from the $d_1$ minimization. Instead of stretching the entire plane in one direction and compressing it in the other, the mechanism is broken down into small sections that slip onto each other to minimize strain. Fig. 2 illustrates graphically how breaking down the plane in strips can reduce the macroscopic change in shape and therefore the strain. Imagine a sheet of metal that has been stretched from its original square shape by an amount corresponding to the Bain strains in the $(001)_\gamma/[[1T0]_\alpha$ plane; its dimensions are now 1.155 by 0.816. By cutting the sheet in strips and by sliding them onto each other, one can obtain a shape that is much closer to the unstretched 1 by 1 sheet, while, locally, the metal in each strip has been stretched by an amount corresponding to the Bain strains. In our proposed mechanism, the strips are 6 atomic layers wide and the actual transformation does not occur in two steps; each strip is distorted through a local shear that occurs simultaneously with the slipping process. At the end of this process, the BCC structure (martensite) is obtained. In order for this mechanism to yield a perfect BCC lattice, each strip needs to slip by an integer number of atomic layers as shown in Fig. 1(c). Filling this condition determines the width of the strips which 6 atomic layers using our choice of lattice parameters. In reality, martensite deviates from perfect BCC depending on the carbon content. We obtain qualitatively similar results if the tetragonal BCT martensite structure is used. It is important to note that this slipping process is fully described by the displacements of the atoms within the transformation cells (Fig. 1). This explains why our algorithm finds unit cell of 6 atoms; each atom in the cell is displaced along the $[11\bar{0}]_\gamma/[[1T1]_\alpha$ direction (blue cell vector) such that the condition is fulfilled at the end of the transformation.

The minimal distance result presented here bears striking resemblance to the PTMT since it involves a slipping process and an invariant plane (discussed further). Moreover, our mechanism naturally yields the correct shear (rotated Bain distortion), the measured habit plane, and orientation relationship, whereas the PTMT requires knowledge of one of the three features to explain the other two. None of those features were implemented a priori in our algorithm, they are all direct consequences of minimizing the distance. The key factor that makes this possible and distinguishes our model from previous works is the addition of the individual atomic displacements inside the cell. The transformation mechanism cannot be fully described by a single distortion matrix because it needs to take into account atomic displacements within the distorted lattice. Moreover, in one of the original PTMT papers [16] and in numerous subsequent studies [11] the $\{112\}_\alpha$ is explicitly used as input, as the lattice invariant shear plane because striations parallel to

FIG. 2. Illustration of the effect of the slipping process. The dashed squares show the undistorted plane and the black rectangle on the left shows that same plane to which the Bain strains of -18.4% and 15.5% are applied. The steps to obtain a shape that is macroscopically similar to the undistorted plane but microscopically similar to the Bain-strained plane are shown from left to right.
that plane (sometimes referred to as Neumann bands) are commonly observed in martensite [3, 14, 28, 29]. The slipping process happens precisely along that plane in our optimal distance mechanism. Because we impose the final structure to be the perfect BCC lattice, our algorithm cannot find the related twinning process as it would lead to a different, twinned BCC lattice. However, by simply inverting the direction of the local displacements of the atoms for one column of unit cells along the [110]γ/[111]α direction as shown in Fig. 3 we can obtain the twinned BCC. This would yield a mechanism very similar to the one presented in Ref. 22 but without the need to assume a particular OR. In that study, researchers also found the \{11\sqrt{6}\} habit plane (discussed later) and found that the twinned and untwinned structures yield two variants of the Kurdjumov-Sachs (K-S) orientation relationship. Additionally, a nearly identical structure where atoms every sixth (112) layers are common to both the twinned and the untwinned lattices as illustrated in the bottom right panel of Fig. 3 have been theorized previously [10].

Using the hard-sphere packing lattice constant, one of the principal strains is exactly zero, therefore, there necessarily exists a plane that is undistorted by the transformation. However, using the experimental lattice parameter, the smallest principal strain is not exactly zero and there does not exist a plane that is fully invariant. The invariant vectors rather form a hyperboloid that approaches the shape of a plane as the smallest principal strain approaches zero. Our approach is to look for a uniformly scaled plane instead of a fully invariant plane. Indeed, there always exists a plane such that the angles between its directions are preserved, i.e., a plane that is similar, in the geometric sense, to the initial plane. Any vector \( \mathbf{u} \) of that plane obey the following equation:

\[
||\mathbf{T}\mathbf{u}|| = k||\mathbf{u}||,
\]  

where \( k \) is a scalar, independent of the choice of \( \mathbf{u} \). Ordering the eigenvalues of \( \mathbf{U} \) such that \( \lambda_1 < \lambda_2 < \lambda_3 \), one can show that the vectors \( \mathbf{u} \) will form a plane if \( k = \lambda_2 \) (see Supplementary Materials). The lattice mismatch between the transformed plane and its equivalent in austenite is \( 1 - \lambda_2 \). In the limit where \( \lambda_2 \to 1 \), which is the case when using the hard-sphere packing lattice constant, the mismatch is zero and the plane is invariant. Using eq. (2), we find that the vector \( \sqrt{2\,0 \pm \sqrt{6}} \) is perpendicular to the invariant plane and it can be expressed in coordinates of the austenite lattice:

\[
\mathbf{n}_{\text{HP}} = P \begin{pmatrix} \sqrt{2} \\ 0 \\ \pm \sqrt{6} \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ \pm \sqrt{6} \end{pmatrix}.
\]  

This plane is approximately 0.5° from the low index (22±5) plane. On the other hand, using the experimental parameters, we find the uniformly scaled plane to be about 0.4° from the low index (22±5) plane with a mismatch of 1.6%. This is an important result since the \{225\}_α habit plane is one of the few experimentally observed habit planes for low alloy plate-like martensite [18, 30]. Moreover, interpreting the uniformly scaled plane as the habit plane allows us to readily obtain the \{112\}_α slipping process as well as the \{225\}_γ habit plane without having to use a dilatation factor or additional shear processes which have been highly criticized by the detractors of the PTMT [30].

Let us now consider that the invariant plane (or more generally, the uniformly scaled plane) is also the habit plane between the two phases. In that case, the rotation \( \mathbf{R} \) is the one for which the invariant plane does not rotate during the transformation. Thus, it must fulfill:

\[
\frac{\mathbf{R}\mathbf{u}\mathbf{v}}{\|\mathbf{R}\mathbf{u}\mathbf{v}\|} = \mathbf{v}.
\]  

Where \( \mathbf{v} \) are unit vectors of the invariant plane. From that relation, using \( \mathbf{U}, \mathbf{P}, \) and \( \mathbf{Q} \) we can calculate the rotation matrix \( \mathbf{R} \). The exact steps necessary to obtain the matrices (one for \( \{1\overline{1}1\} + \sqrt{6} \) and one for \( \{1\overline{1}1\} - \sqrt{6} \)) are detailed in the Supplementary Materials. Finally, the orientation relationship is given by the transformation matrix that changes the basis from FCC to BCC. Let us transform some vector \( \mathbf{d}^{(γ)} \) from the FCC basis to the BCC basis: \( \mathbf{R}^T \) transforms the vector into the unrotated FCC basis, \( \mathbf{P}^T \) converts it to the eigenvalue basis and finally \( \mathbf{Q} \) converts it from the eigenvalue basis to the BCC basis. Hence:

\[
\mathbf{d}^{(α)} = \mathbf{Q}\mathbf{P}^T\mathbf{R}^T\mathbf{d}^{(γ)}
\]  

By setting \( \mathbf{d}^{(γ)} = [1\overline{1}1]_γ \) and using the first invariant plane (\( \{1\overline{1}1\} + \sqrt{6} \)), we get \( \mathbf{d}^{(α)} = [0 - \sqrt{3/2} \sqrt{3/2}]_α \).
which is parallel to $[0\bar{1}1]_\alpha$ and by setting $d^{(\gamma)} = [110]_\gamma$ we get $d^{(\alpha)} = [-\sqrt{2/3}, \sqrt{2/3}, \sqrt{2/3}]_\alpha$ which is parallel to $[\bar{1}11]_\alpha$. In other words, we find the following OR: $[110](1\bar{1}1)_{\gamma} / [\bar{1}11](0\bar{1}1)_{\alpha}$ which is a variant of the K-S OR: the most commonly observed OR in plate-like martensite. Similarly, using the other invariant plane ($\{1\bar{T}-\sqrt{6}\}$), we get: $[110](\bar{1}11)_{\gamma} / [\bar{1}T1](10\bar{1})_{\alpha}$ which is another variant of the K-S OR. With the experimental lattice parameter, we find the same orientation relationship with a misalignment between the $\{111\}_\gamma$ and $\{011\}_\alpha$ planes of less than 0.4°.

During the martensitic transformation in bulk materials, austenite does not fully transform into martensite; the two phases coexist after the transformation. Therefore, there is no habit plane and no constraint on the relative orientation of the two structures. In that case, $T = U$ such that there is no rotation component in the deformation. In other words, the mechanism is the same but the strain directions do not rotate during the transformation which makes it the true mechanism of minimal distance. In that case ($T = U$) the OR is given by:

$$d^{(\alpha)} = QP^Td^{(\gamma)}$$  \hspace{1cm} (8)

Which leads to the $[001](110)_\gamma / [\bar{1}10](\bar{1}11)_\alpha$ orientation relationship, which represents a variant of the Pitsch OR. This explains why it is the Pitsch OR (and not the K-S OR) that is observed experimentally in thin films [7, 9].

In conclusion, we showed how minimizing the distance travelled by all atoms from the austenite to the martensite phase in steels provides a description of the martensitic transformation. It can explain all the key experimentally observed features without relying on any experimental input (except lattice constants) and without any adjustable parameters. Moreover, we also show how our description provides a unifying framework for most of the previously theorized mechanisms thereby offering a solution to the longstanding and important problem of finding a general description of the martensitic transformation. Lastly, our results reaffirm the principle of distance minimization as a governing principle when describing diffusionless, solid-solid phase transformations.

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