Supplementary Material for Characterization of Grain Boundary

Disconnections in SrTiO$_3$ Part I: The Dislocation Component of Grain Boundary

Boundary Disconnections

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$^*$Conducted when the author was at (5)
$^{**}$Conducted when the author was at (4)

Introduction

Grain boundaries are often described using geometric methods. Special boundaries of high symmetry are usually described using the coincident site lattice (CSL) theory [1]. According to the displacement shift complete (DSC) lattice model [2], high angle grain boundaries can be treated as small deviations from the nearest CSL boundary, accommodated by secondary (grain boundary) dislocations.

The DSC lattice can be defined as the lattice of difference vectors between the two lattices of the grains creating the boundary. The DSC lattice vector ($d^\text{DSC}$) can be found graphically by defining the smallest displacements required to restore the dichromatic pattern (a schematic pattern showing atomistic positions of two lattices). Mathematically, $d^\text{DSC}$ is defined as

$$d^\text{DSC} = x^{(2)} - x^{(1)} = (I - A^{-1})x^{(2)} \quad (1)$$
where $A$ is a transformation tensor which relates the coordinate systems of both grains, and can be used to transform vector $x^{(2)}$ in lattice 2 to vector $x^{(1)}$ in lattice 1:

$$x^{(2)} = Ax^{(1)}. \quad (2)$$

A displacement of one crystal with respect to the other by a DSC lattice vector restores the dichromatic pattern, but with shifted coincidence sites, and thus the resulting CSL is shifted [1,3,4].

Steps and dislocations along grain boundaries can be described using the DSC model. The Burgers vector $b$ and step vectors $s_1$ and $s_2$ in the two lattices are related by

$$b = s_1 - s_2 \quad (3)$$

The step height is determined by multiplying the step vector by a unit vector $n$ normal to the grain boundary plane. A pure step gives $b = 0$ and $s_1 n = s_2 n = 0$ holds for a pure dislocation [1,2,3].

When applying the DSC terminology into the disconnection model, the dislocation character of the disconnection is defined by a Burgers vector which can be found from the difference of the translation component of the steps in each grain expressed in the coordinate system of one of the grains, according to (4), where $P$ is the coordinate transformation matrix relating the crystal lattices in a reference system which does not contain the defect, and which transforms a vector in the $\mu$ grain, $t_\mu$, into a vector in the $\lambda$ grain, $t_\lambda$ (similar to (3))

$$b = t_\lambda - Pt_\mu \quad (4)$$

Another method for describing the dislocation component of a disconnection is by drawing a circuit around the disconnection and expressing the Burgers vector as the difference in the total paths in each grain. In the coordinate system of one of the grains (e.g. the $\lambda$ grain) the Burgers vector is
where \( C_\lambda \) and \( C_\mu \) are the paths in each of the two grains. The step term of the disconnections can be characterized by the height of the step, expressed by multiplying the translation component of the steps by a unit vector normal to the grain boundary plane [5,6,7,8,9].

In many cases the Burgers circuit drawn around a defect is compared to a defect free reference system. Thus a complete circuit is drawn around a defect, and then the circuit is transferred into the reference system. The difference in the start and end points in the reference system is the Burgers vector associated with the defect. This method takes into account all possible symmetry operations, not only translation, as suggested in equation (4), and can be applied at interfaces and in the bulk [5,9].

**Results**

**The Dislocation Component of the Disconnections in the Boundary Presented in Case Set 1 in the Manuscript**

To characterize the dislocation component of the disconnections along the boundary in Figure 1b in the manuscript, the transformation matrix \( P \) which transforms a vector in the coordinate system of the left grain into the coordinate system of the right grain, was found based on the coordinate systems marked in Figure S1. Due to the low symmetry of the boundary (which is demonstrated in Figure S3 and discussed below), the origin of both coordinate systems was taken as the same point in space for the calculation of \( P \). The translation of the origin points can be added separately if needed. It should be noted that this translation between the origin of
both coordinate systems (taken at a certain constant position within a unit cell in each grain, for example) has varying values due to the low symmetry of the boundary.

An angle of $14.3^\circ$ was measured between the [010] direction in the right grain and the [011] direction in the left grain, and $12.4^\circ$ between the $[100]$ direction in the right grain and the $[100]$ direction in the left grain. Even though the left grain deviates from the $[011]$ zone-axis by a small angle, this was neglected in the following analysis and both grains were considered to be in a low-index zone-axis. The resulting $P$ matrix is

$$
P = \begin{pmatrix}
-\cos 12.4 & \frac{\sin 14.3}{\sqrt{2}} & \frac{\sin 14.3}{\sqrt{2}} \\
\sin 12.4 & \frac{\cos 14.3}{\sqrt{2}} & \frac{\cos 14.3}{\sqrt{2}} \\
0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}
\end{pmatrix} \approx \begin{pmatrix}
-1 & 0.2 & 0.2 \\
0.2 & 0.7 & 0.7 \\
0 & 0.7 & -0.7
\end{pmatrix}
$$

I. Burgers Circuits

In this section the dislocation component of the disconnections will be characterized using several approaches available in the literature regarding Burgers circuits, where we show that such analysis fail for general high angle grain boundaries. In order to draw a Burgers circuit, the boundary must be crossed twice. The easiest possibility to cross the boundary is by opposite vectors canceling each other. Since exact opposite vectors can’t be found based on the atomistic structure of the boundary (due to the secondary grain boundary dislocations along the boundary), two vectors were selected, such that they are as close as possible to being opposite to each other. Four such possibilities for circuits are drawn in Figure S1a-d. In these cases, the Burgers vector can be found from the difference in the total paths traveled in each grain.
described in the coordinate system of one of the grains. Since the vectors crossing the boundary were selected to be as close as possible to canceling each other, the transformation matrix \( P \) is applicable in addition to equation (5) (without corrections related to the translations between the origin of the coordinate systems, taking into account a point of near coincidence between the coordinate systems of both delimiting grains along the boundary).

If we consider the circuit A-H in Figure S1a (drawn with white lines), the total distance travelled in the left grain is BC which is \(-6[011]\), and the total distance in the right grain is \([140]\), as summarized in Table S1. These distances do not depend on the path selected for the circuit; different paths starting and ending at the same points (points E and H in the right grain and points A and D in the left grain) yield the same total path. For example, one might consider replacing \( C_A \) in the white circuit with the orange path drawn which, as expected, yields the same total path in the right grain.

By using (5) the resulting Burgers vector is \( b_A = [1.1 \ 4.2 \ 0] \) defined in the coordinate system of the right grain. It should be noted that since the vectors crossing the boundary were selected such that they are as close as possible to being opposite to each other (rather than cancelling each other), the remaining difference between the two should be added to the Burgers vector found above. Since these differences were intentionally made to be as close to zero as possible we neglect them in this work. The calculated value of the Burgers vector is the sum of the dislocations enclosed in the circuit, since single dislocations cannot be addressed (as will be described below).
When considering the white circuit I-R in Figure S1b, the total distances traveled in each grain are summarized in Table S2. As such, the resulting Burgers vector is $b_b = [1.7 \ 6.6 \ 0]$ defined in the coordinate system of the right grain.

Doing the same procedure on the circuits drawn in Figure S1c and Figure S1d (the total distances traveled in each grain are summarized in Table S3) we obtain $b_c = b_d = [1.5 \ 4.8 \ 0]$

It can be seen that when a circuit surrounds the same number of steps which are of similar length and height, the resulting Burgers vector is the same regardless of the exact position of the circuit. When the number of steps incorporated in a circuit changes, or the nature of the steps themselves changes, the resulting Burgers vector changes. It should be noted that small differences between $b_c$ and $b_d$ are expected to occur due to the small differences between the two vectors crossing the boundary in each case, which almost cancel each other (resulting from the mismatch along the boundary), and are neglected in this work. In the circuits used to calculate $b_c$ and $b_d$, in addition to selecting vectors crossing the boundary to be as close as possible to canceling each other, the position of the circuits was selected such that they are close to each other. This was done to keep the differences between the position of columns of atoms required to define the vectors crossing the boundary in each circuit of the same order of magnitude. As will be discussed below, due to the low symmetry of the boundary and the grain boundary dislocations, these differences change along the boundary within possible large representative unit cells. As such, significant changes in the position of two circuits with the same $C_{\mu}$ and $C_{\lambda}$ (even when incorporating the same number of steps of the same nature) can cause significant changes in the difference between the two vectors crossing the boundary in each circuit, such that in some cases this difference can be non-negligible.
Since the boundary should be crossed twice in regions which are identical in order for them to cancel each other, such a circuit can only start and end at certain positions along the boundary. In the case of the boundary presented in Figure S1, four such possibilities were drawn, resulting in Burgers vectors which vary, depending on the position of the start and end point of the circuit, due to the different number and nature of steps and grain boundary dislocations enclosed within each circuit. Within the limits of using opposite vectors to cross the boundary, the Burgers circuit cannot be as small as needed to define individual disconnections with a step component or individual secondary dislocations. Within any selected circuit only the sum of secondary dislocations can be found using this method.

For all of the Burgers vectors determined above, the Z component (which adds a screw component to the dislocations) vanishes. Since the boundary is crossed twice by vectors which are as close as possible to canceling each other, we assume that the Z component is also (almost) cancelled. However, a small residual Z component is expected due to the small deviation of the grain on the left from the [011] zone-axis, and the difference between the vectors crossing the boundary.

The Burgers vector can also be found by drawing the same closed circuits defined above on a reference system at the grain boundary which is free of disconnections. The difference between the start and end points is the Burgers vector. When applying the circuits drawn in Figure S1a-d into a reference system (neglecting the vectors which cross the boundary as they were intentionally set to cancel each other in circuits a-d), the same paths will appear since no significant changes in the atomistic structure from that of bulk SrTiO$_3$ were detected in the boundary area (within the limitations of the STEM data). Since the reference system has the same structure as the experimental data, the resulting Burgers vectors would vanish. In practice,
the difference between the vectors crossing the boundary and the small possible changes in the atom positions (which were not taken into account here) will yield small Burgers vectors.

It should be noted that while it is convenient to cross the boundary using (opposite) vectors which then cancel, it is possible to use different vectors, which are both expressed in the same coordinate system used to find the resulting Burgers vector. Figure S2 demonstrates two circuits which include one step from the left grain (I’-P’ and Q’-X’) and two other circuits which include one step from the right grain (I”-P” and Q”-X”). In each pair of circuits, the paths traveled in each grain are identical. The total distances traveled in each grain in circuits I’-P’ and Q’-X’ in Figure S2 are summarized in Table S4. In all cases the pair of vectors crossing the boundary in each circuit are not opposite and thus don’t cancel each other. In each circuit different vectors crossing the boundary are required, according to the structure of the boundary, due to the changes in the position of the coordinate systems along the boundary (resulting in grain boundary dislocations). By expressing the sum of the vectors crossing the boundary in each circuit in the coordinate system of the right grain in order to add it to the expression resulting from (5), different values are extracted in each circuit, even though each pair of circuits expresses a single step in one of the grains. This is the outcome of the Burgers vectors along the boundary being the result of the two types of disconnections (steps and grain boundary dislocations which are not distributed uniformly). As such, even by using Burgers circuits which enclose one step using the same paths in each of the grains and suitable vectors crossing the boundary (which don’t cancel), different Burgers vectors will be extracted at different positions along the boundary, apparently due to the non-uniformity of the second type of disconnection (the grain boundary dislocations) located along the boundary. These dislocations can be found using the DSC lattice and will be addressed below.
As such, in general high-angle grain boundaries, where the atomistic structure of the boundary can be found, specific vectors crossing the boundary can be used but the resulting Burgers vector is the sum of the secondary dislocations at the boundary. The Burgers vector of such secondary dislocations (disconnections) cannot be found using the circuit. Thus, the use of vectors crossing the boundary which don’t cancel only defines sums of dislocations without the ability to find the Burgers vectors related to one disconnection (either a step or a secondary grain boundary dislocation).

Another restriction to this method is that the circuit cannot cross a step as a step is part of the disconnection which is being characterized. Thus, the circuit must start and end at grain boundary planes. It should be noted that in the general case the atomistic structure of general boundaries cannot be found and thus the circuit method cannot be used at all. As such, using a Burgers circuit to find the Burgers vectors of the dislocation component of the disconnection offers a limited amount of information for general high-angle grain boundaries.

II. Translation Vectors

In this section the dislocation component of the disconnections will be characterized using translation vectors, where we show that such analysis fails for general high angle grain boundaries. When defining the Burgers vector by the translation vectors of the steps from both sides using (4), we obtain $b = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} - P \begin{bmatrix} 0.5 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 1.5 \\ 0.9 \\ 0 \end{bmatrix}$. It should be noted that this approach does not take into account grain boundary dislocations and their influence on the disconnections, which can result in varying shifts between the origin of the coordinate systems of both grains. In addition, the steps from both sides originate at different positions along the boundary, in a
manner that is not uniform along and across the boundary. As such, the distances between steps from both sides vary along the boundary (as well as the mismatch between steps and thus the grain boundary dislocations) and different Burgers vectors should result. Thus, since the steps from both sides do not start at the same starting point and can have varying distances between their positions, this analysis fails. The specific calculated value was extracted using the calculated P matrix which takes into account a common origin for both coordinate systems, which is not the case in this boundary, and the same starting point for both translation vectors, as usually done when this method is applied.

However, applying the actual transformation matrix (which takes into account the local translations between the coordinate systems of both grains) will still not yield different Burgers vectors for the case of disconnections composed of steps from both grains. This is due to the fact that this method does not take into account different possible distances between the steps, and requires the same starting point for both translation vectors. Adding the local translation between the origin of the coordinate systems will not be representative of the boundary, and will require an additional varying component to account for the position of the steps.

As discussed above, due to the varying changes in the positions of the translation vectors along the boundary, the calculation mentioned in (4) fails, and the translation between pairs of two steps from each side should be taken into account. This results in the absence of sums of secondary grain boundary dislocations which are present along the boundary between the disconnections (with a step component), which are expected to be included in the end result.

III. The DSC (Displacement Shift Complete) Lattice
In this section the dislocation component of the disconnections will be characterized using the DSC lattice, where we show that such analysis fails for general high angle grain boundaries. The dichromatic pattern of the boundary in Figure 1 in the manuscript is depicted in Figure S3. Due to the STEM distortions, the dichromatic pattern was constructed using the upper most rows of unit cells in the atomistic solution indicated in Figure 1b in the manuscript. As a result, the dichromatic pattern may contain an intrinsic error. The error is associated with STEM distortions and is estimated to be of the order of half an Angstrom or less. An error of that magnitude is insignificant in defining the discernible component of the dislocation character of the disconnection, as will be shown below.

From the dichromatic pattern presented in Figure S3, no structural representative unit cell was found to describe the dichromatic pattern in a periodic manner. Lines (in red and blue) were drawn to distinguish atom sites in both grains which are in similar positions. The lines in one color distinguish positions of atoms from both grains which are in similar positions in space. Since in this large volume (embedded inside the cells marked in one color) small deviations in the positions of the marked atom sites are still apparent, the structural unit cell of the dichromatic pattern will include a larger volume and many more atoms. The lack of a simple unit cell in the dichromatic pattern is the result of the low symmetry of the boundary, which includes shifts in atom positions in all dimensions as demonstrated in the transformation matrix calculated above. This is the result of the variation in the relative positions of the origins of both coordinate systems (secondary grain boundary dislocations). Thus, the translation between the two coordinate systems is not uniform and has components in all dimensions. A repetitive appearance of the translation between the coordinate systems will occur between similar positions within unit cells of the dichromatic pattern, which will include many unit cells of each grain.
As such, the DSC unit cell cannot be found graphically for this boundary (by finding the smallest distances required to restore the dichromatic pattern). The DSC lattice can be found mathematically using (1), where the matrix $A$ is in practice the sum of matrix $P$ and a matrix which defines the shifts in the origin of the coordinate systems (resulting from the grain boundary dislocations). Thus, we obtain:

$$d^{DSC} = \left[ \begin{array}{ccc} 2 & -0.2 & 0 \\ -0.2 & 0.3 & -0.7 \\ -0.2 & -0.7 & 1.7 \end{array} \right] + \left[ \begin{array}{ccc} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{array} \right] x^{(2)}.$$

In order to use this calculation, the position of pairs of atoms (one from each grain), of which the translation by a $d^{DSC}$ between them would restore the dichromatic pattern, should be known. As discussed previously, such pairs of atoms cannot be found due to the low symmetry of the boundary.

It should be noted that while the DSC lattice positions are not necessarily occupied by atoms, atom positions must occupy positions in the DSC lattice. As such, if we consider the atoms within the rectangles marked in Figure S3b as parts of the DSC unit cell, the DSC lattice of this boundary will include many lattice points with varying distances allowing for many Burgers vectors to appear (since the Burgers vectors should be composed of the DSC dense lattice lines). The Burgers vectors can be calculated using (3), and this resulted in $[1.5 \ 0.9 \ 0]$ expressed in the coordinate system of the right grain, as mentioned above. Since the step vectors in both grains do not originate at the same position as required for the use of (3) (due to varying changes in the origins of the coordinate systems and the varying positions of the steps along the boundary), this value does not represent the actual Burgers vector. In addition, since the resulting DSC unit cell will be large containing many positions, this boundary does
not represent all the general trends in the SrTiO$_3$ system. This method can only be used when the atomistic structure of the boundary is known, which is not the case for most general grain boundaries. As demonstrated in Figure S3, even when the atomistic structure of the boundary is known and the DSC lattice can (theoretically) be found, the boundary results in many DSC lattice points with low symmetry, indicating that the DSC unit cell is large and not representative.

Comments About Grain Boundary Dislocations and Strain

In this work grain boundary dislocations are characterized as a separate type of disconnections, while Pond et al. [8] refer to them as a product of the disconnections which also have a step character. Whenever a disconnection with both a step and a dislocation component is present along a boundary, there is a change between the atomistic structure along the boundary planes on both sides of the disconnection. If, for example, the atoms along the grain boundary plane on one side of such a disconnection coincide, grain boundary dislocations will form at the other side of the disconnection. If the atoms don’t coincide on both sides of such a disconnection, a change in the grain boundary dislocations will occur (type and density) due to the presence of such a disconnection. This results in different grain boundary dislocations on both sides of such a disconnection. This is an inherent result from a disconnection with a step and a dislocation component, and thus the grain boundary dislocations resulting from such a disconnection (if the atoms coincide in one side of the disconnection, or the change in the grain boundary dislocations, if the atoms from both sides don’t coincide) can be correlated to the disconnection.

The frequent appearance of a variety of such disconnections in a non-uniform manner in Figure S1 (and Figure S2) results in frequent changes in the grain boundary dislocations along the
boundary. As such, the grain boundary dislocations change after every step along the boundary, and therefore, many types of grain boundary dislocations are present along the boundary. In this boundary, the atoms along the grain boundary planes never coincide along the boundary, and thus we can only refer changes in the grain boundary dislocations to a disconnection. Since the grain boundary dislocations are frequently changing by the three types of disconnections with step character (even due to the existence of a disconnection composed of a step in one grain and a grain boundary plane in the second grain), and the boundary is of low symmetry (thus grain boundary dislocations are expected), we refer to them separately in the paper as a distinct type of disconnection with no step component.

We assume that grain boundary dislocations would exist close to a disconnection with a step component, and would decay after some distance by the tendency of the material to prefer low energy 2D structures along grain boundary planes (or in other words, to reduce the total energy by eliminating the excess of energy related to strain). Thus, we expect that a certain type of grain boundary dislocation would be preferred at a distance from a disconnection with a step component. These grain boundary dislocations would then lie along the segments of grain boundary plane and their nature would depend on the local distance between the origins of the coordinate systems of both grains (which adds translation vectors to the burgers vectors calculated for example by the circuit method, as detailed above). As such, if the decay length is shorter than the length of the grain boundary plane (between two relevant disconnections), the existence of a disconnection with a step and a dislocation component creates a second type of grain boundary dislocation. If the decay length is longer than the length of a grain boundary plane (between two relevant disconnections), then the grain boundary dislocations change into another type, regardless of any low energy structures away from the disconnection. As such, the grain boundary dislocations are not periodic along the boundary.
Comments on the Atomistic Structure of the Boundary in Figure 1 in the Manuscript

In Figure S4 QSTEM simulations of both delimiting grains of the boundary in Figure S1 (and Figure S2) are presented as a function of thickness (all other parameters were kept constant as dictated by the microscope). It can be seen that a contrast reversal occurs above thickness of about 80nm in the grain on the right. For both grains heavy atoms are represented by bright contrast. A contrast reversal for the simulation of the left grain was not noted up to a sample thickness of about 100 nanometers. As such, the relevant pair of simulations must be for a thickness which is blow 80 nm. A thickness of about 30 nm was selected to be presented in the paper due to the enhanced contrast.

References


### Tables

**Table S1:** Geometrical description of the Burgers circuit drawn in white in Figure S1a.

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<th>$C_\mu$</th>
<th>$C_\lambda$</th>
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<td>2[100]</td>
<td>EF</td>
</tr>
<tr>
<td>BC</td>
<td>-6[011]</td>
<td>FG</td>
</tr>
<tr>
<td>CD</td>
<td>-2[100]</td>
<td>GH</td>
</tr>
<tr>
<td>Total</td>
<td>-6[011]</td>
<td>Total</td>
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**Table S2:** Geometrical description of the Burgers circuit drawn in white in Figure S1b.

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</tr>
<tr>
<td>JK</td>
<td>-10[011]-0.5[010]</td>
<td>OP</td>
</tr>
<tr>
<td>KL</td>
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<td>PQ</td>
</tr>
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<td>QR</td>
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<tr>
<td>Total</td>
<td>$\frac{1}{2}$ 21 21</td>
<td>Total</td>
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</table>

**Table S3:** Geometrical description of the white Burgers circuits drawn in Figure S1c and the in Figure S1d.

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<td>WX or E<code>F</code></td>
</tr>
<tr>
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<td>-7[011]</td>
<td>XY or F<code>G</code></td>
</tr>
<tr>
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<td>YZ or G<code>H</code></td>
</tr>
<tr>
<td>Total (SV or A<code>D</code>)</td>
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<td>Total (WZ or E<code>H</code>)</td>
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Table S4: Geometrical description of the dashed white Burgers circuits drawn in Figure S2.

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<td>M’N’ or U’V’</td>
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</tr>
<tr>
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<td>N’O’ or V’W’</td>
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<td>O’P’ or W’X’</td>
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<td>Total (M’P’ or U’X’)</td>
<td>2[010]</td>
</tr>
</tbody>
</table>
Figure Captions

Figure S1: (a-d) Burgers circuits across the boundary presented in Figure 1 in the manuscript. The distortions in the atomistic model shown in the micrograph were omitted from the analysis. The coordinate systems of each grain are marked on the micrograph.

Figure S2: Burgers circuits including one step each across the boundary presented in Figure 1 in the manuscript.

Figure S3: (a) The dichromatic pattern of the boundary presented in Figure 1 in the manuscript, and (b) with overlaid lines which represent positions of atoms from both grains which are placed in similar positions. For clarity, the edges of unit cells of both grains are marked by the black and light blue lines.

Figure S4: QSTEM simulations of the delimiting grains of the boundary presented in Figure S1 and Figure S2 and Figure 1 in the manuscript. The thickness of the simulated specimen is stated on the left of the simulations. The simulations were prepared using a convergence angle of 29.9mrad, a source size of 0.7angstrom, accelerating voltage of 200kV, Cs=1μm, and a detector with inner and outer collection angles of 80-200 mrad.