Appendix A. The TM methodology for a twin in a simple cubic lattice

Figure A1a illustrates the methodology of the TM for a (103) twin in a simple cubic, $\Sigma 5$ crystal. The plane of twin symmetry is shown as a solid line. The CDP is shown in Fig. A1b. Inspection of the CDP reveals that the probable disconnection has $h = 3h_0$ with **b** as shown. The Burgers vector $when\, h = h_0$ has an elastic energy $\propto b^2$ that is four times as large. The Burgers vector is smaller for $h = 2h_0$ but the shuffle vectors are large, so it would be difficult to nucleate. For $h = 3h_0$, both **b** and *h* are relatively small. For this example, the CDP and the CDC coincide. The dividing surface, the solid line in Fig. A1b, is located midway between the last twin plane transformed and the next untransformed matrix plane. It is displaced by *d*/2 from the coherent interface in the CDC to the red position, where *d,* here equal to h_0 is the interplanar spacing (the twin symmetry plane, dashed line, remains the coherent plane). Matrix atoms are removed below the dividing surface and twin planes are removed above the dividing surface, creating the Bilby bicrystal (Hirth et al. 2013), which also has an interface displaced from atomic planes by *d*/2. This interface corresponds to the thermodynamic Gibbs interface.

The former matrix atoms must undergo added displacements so that the crystal structure is correctly that of the twin. This is accomplished by the shuffles. Shuffles are local atom rearrangements that produce no plastic strain but which complete a transformation. In the CDC, the displacements are $\mathbf{u}^0(\lambda)$ and $\mathbf{u}^0(\mu)$. The shuffle vectors $\mathbf{s}_1$ and $\mathbf{s}_2$ (which quantify the displacements associated with the rearrangement of atoms) for the (103) twin are depicted in Figs. A1b and A1c. These vectors are of the exchange type. As noted in Section 2.2, the shuffles are related to the displacements in the CDC by $\mathbf{s} = \mathbf{u}^0(\lambda) - \mathbf{b}$. Figure A1c demonstrates the SDC for the (103) twin. In the SDC, the displacements are $\mathbf{u}(\lambda)$ and $\mathbf{u}(\mu)$, and the shuffles are given by $\mathbf{s} = \mathrm{u}(\lambda)$. The matrix above the dividing surface is already sheared by **b** in this diagram.

Physically, if a disconnection moves along the interface, the entire matrix above the interface is shifted by the Burgers vector. This is represented in a schematic view of the real crystal in Fig. A2. Above the red line in Fig. A1b, that is all that happens. Between the dark and red lines, the matrix has been converted to the twin. Thus, the matrix atoms are displaced to the left by **b** in region B while atoms in region A are not displaced. Atoms are also displaced in region C. However, this leaves the structure in this little region in incorrect positions. Shuffles are required in region C to complete the twinning transformation. Hence, disconnection motion requires both shear and shuffles, creating a perfect twin increment in its wake.

To connect to the mineral applications, Fig. A1 could represent reference spaces for structural groups in a complex cubic crystal.

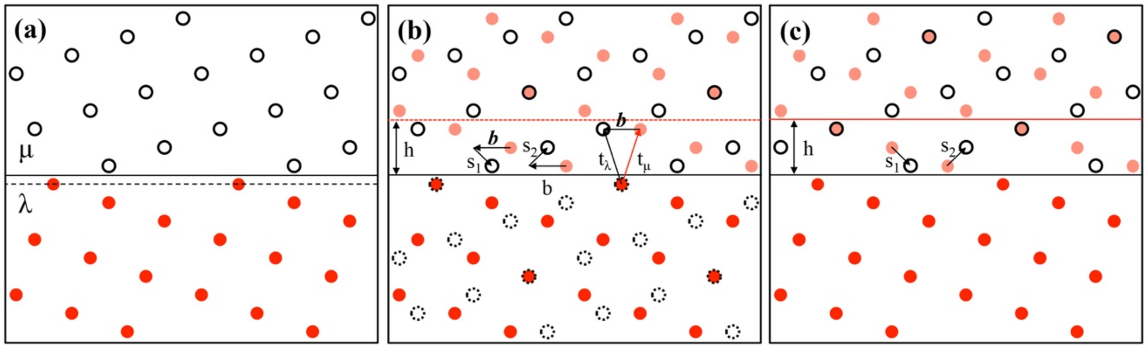

Figure A1. (**a**) Ideal Bilby bicrystal for a (103) twin in a simple cubic structure. The position of the interface is shown as solid line. (**b**) Corresponding CDP/CDC for a $h = 3h_0$ disconnection is depicted, along with associated **b** and **s** vectors. Position of dividing surface shown as solid line, resultant twin symmetry plane by dashed line. (**c**) Shifted SDC with the μ structure shifted by **b** relative to λ. The **s** vectors are the same as those in **b**.

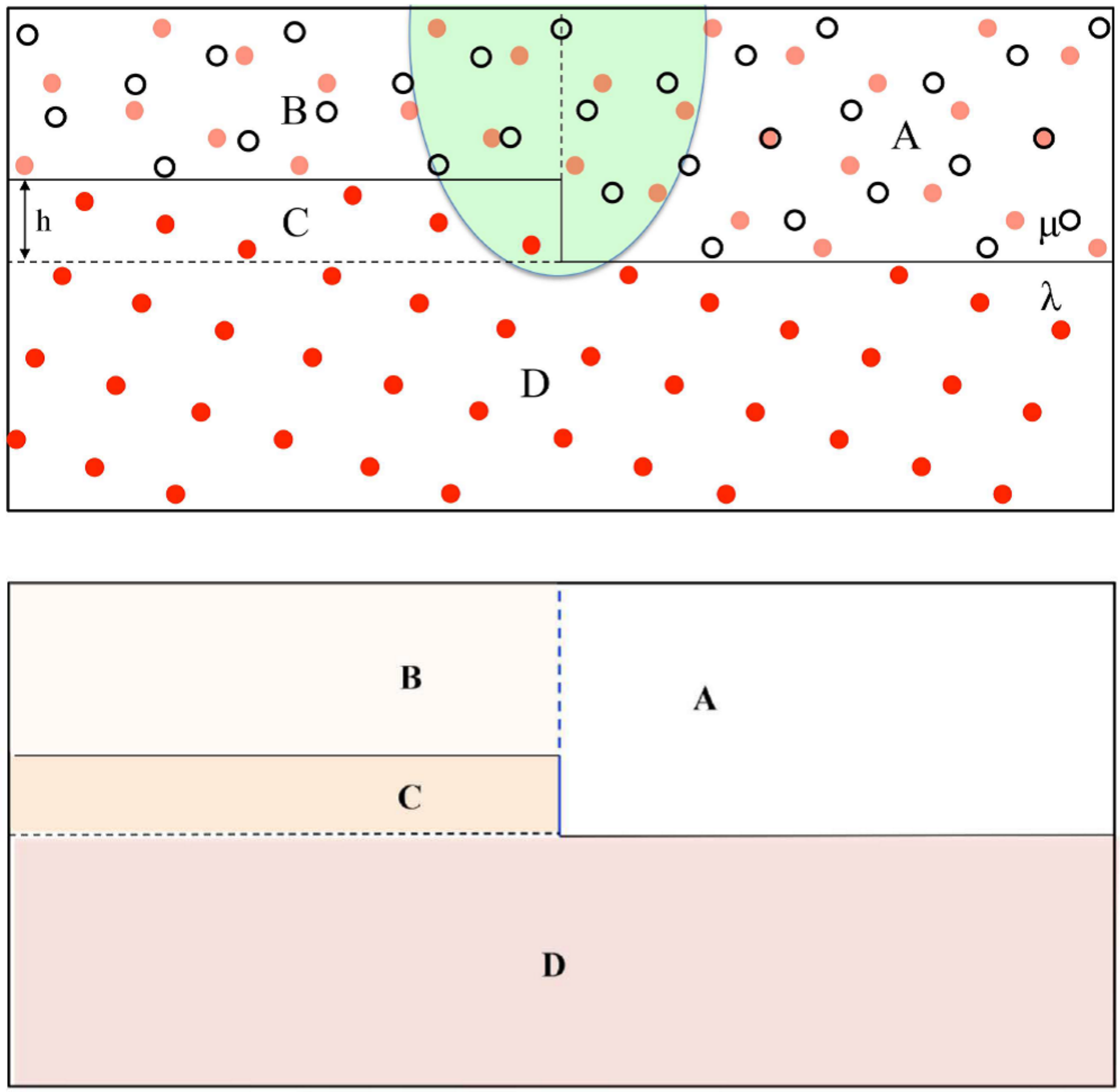

Figure A2. (**a**) Schematic of disconnection traversing the twin. The disconnection with $h = 3h_0$ moves to the right and converts region C from matrix A to twin C, growing twin D. In the wake of the defect. the matrix region B is displaced by **b**. In region C the matrix is displaced by a combination of shear by **b** and shuffles **s**.