International Tables for Crystallography (2006). Vol. D, Figure 3.3.8.1, p. 419.

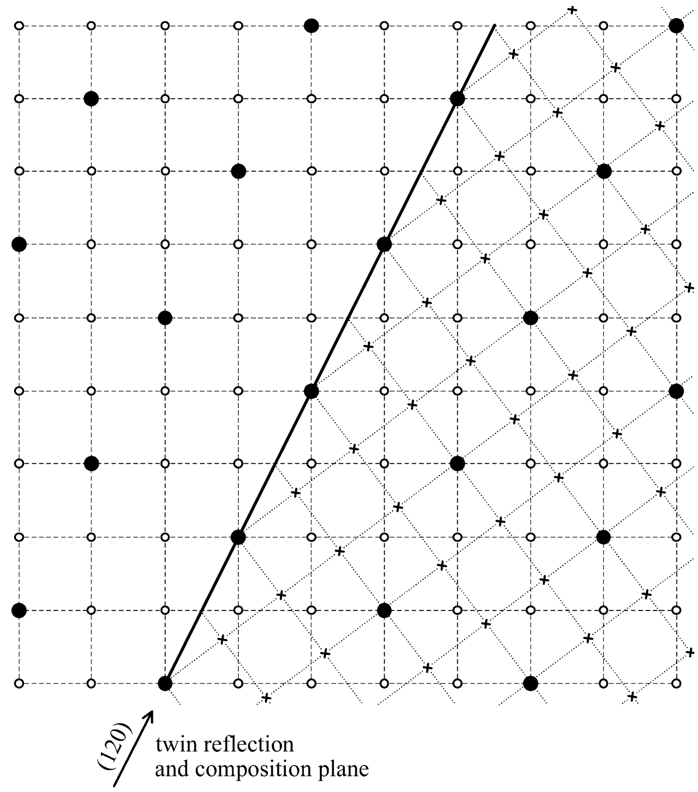

Fig. 3.3.8.1. Lattice relations of Σ5 twins of tetragonal crystals with primitive lattice: twin mirror plane and composition plane (120) with twin displacement vector **t = 0**. Small dots: lattice points of domain 1; small x: lattice points of domain 2; large black dots: Σ5 coincidence lattice.

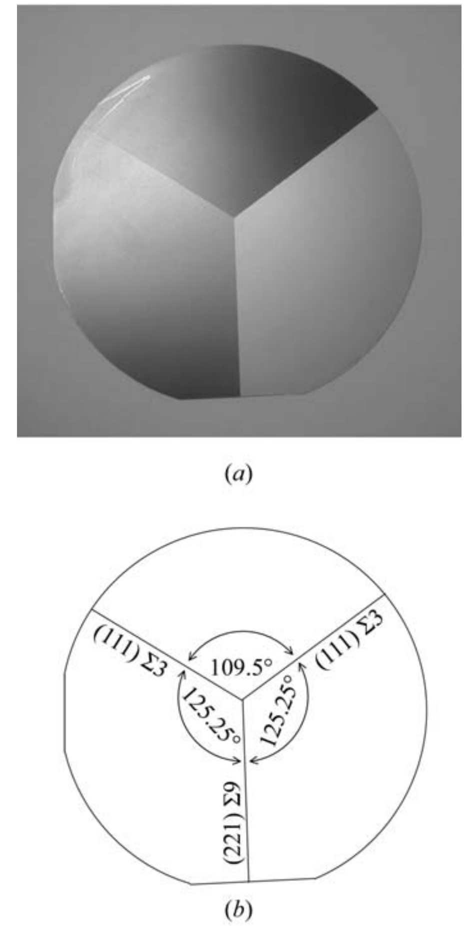

Fig. 3.3.8.2. (*a*) A (110) silicon slice (10 cm diameter, 0.3 mm thick), cut from a Czochralski-grown tricrystal for solar-cell applications. As seed crystal, a cylinder of three coalesced Si single-crystal sectors in (111) and (221) reflection-twin positions was used. Pulling direction [110] (Courtesy of M. Krühler, Siemens AG, München). (*b*) Sketch of the tricystal wafer showing the twin relations [twin laws *m*(111) and *m*(221)] and the Σ characters of the three domain pairs. The atomic structures of these (111) and (221) twin boundaries are discussed by Kohn (1956, 1958), Hornstra (1959, 1960) and Queisser (1963).

to $[j] = 13$. Later structural studies, however, suggest the possibility of disorder instead of twinning.

(4) *Galena, PbS* (NaCl structure). Galena crystals from various localities often exhibit lamellae parallel to the planes {441} which are interpreted as (441) reflection twins with $[j] = 33$ (Σ33 twin) (*cf.* Niggli, 1926, Fig. 9k on p. 53). These natural twins are deformation and not growth twins. In laboratory deformation experiments, however, these twins could not be generated. A detailed analysis of twinning in PbS with respect to plastic deformation is given by Seifert (1928).

(5) For cubic metals and alloys *annealing twins* (*recrystallization twins*) with $[j] > 3$ are common. Among them *high-order twins* (*high-generation twins*) are particularly frequent. They are based on the Σ3 (spinel) twins (first generation) which may coalesce and form 'new twins' with $\Sigma 9 = 3^2$ [second generation, with twin reflection plane (221)], $\Sigma 27 = 3^3$ [third generation, twin reflection plane (115)], $\Sigma 81 = 3^4$ [fourth generation, twin reflection plane (447)] *etc.* Every step to a higher generation increases Σ by a factor of three (Gottstein, 1984). An interesting and actual example is the artificial silicon *tricrystal* shown in Fig. 3.3.8.2, which contains three components related by two (111) reflection planes (first generation, two Σ3 boundaries) and one (221) reflection plane (second generation, one Σ9 boundary).

(6) The same type of tricrystal has been found in cubic magnetite (Fe_3O_4) nanocrystals grown from the biogenic action of magnetotactic bacteria in an aquatic environment (Devouard *et al.*, 1998). Here, HRTEM micrographs (Fig. 6 of the paper) show the same triple-twin arrangement as in the Si tricrystal above. The authors illustrate this triple twin by (111) spinel-type intergrowth of three octahedra exhibiting two Σ3 and one Σ9 domain pairs. The two Σ3 interfaces are (111) twin reflection planes, whereas the Σ9 boundary is very irregular and not a compatible planar (221) interface (*i.e.* not a twin reflection plane).

(7) A third instructive example is provided by the fivefold cyclic 'cozonal' twins (zone axis $[1\bar{1}0]$) of Ge nanocrystals (Neumann *et al.*, 1996; Hofmeister, 1998), which are treated in Section 3.3.10.6.5 and Fig. 3.3.10.11. All five boundaries between neighbouring domains (sector angles 70.5°) are of the Σ3(111) type. Second nearest (2 × 70.5°), third nearest (3 × 70.5°) and fourth nearest (4 × 70.5°) neighbours exhibit Σ9, Σ27 and Σ81 coincidence relations (second, third and fourth Σ generation), respectively, as introduced above in (5). These relations can be described by the 'cozonal' twin reflection planes (111), (221), (115) and (447). Since 5 × 70.5° = 352.5°, an angular gap of 7.5° would result. In actual crystals this gap is compensated by stacking faults as shown in Fig. 3.3.10.11. A detailed treatment of all these cases, including structural models of the interfaces, is given by Neumann *et al.* (1996).

(8) Examples of (hypothetical) twins with $[j] > 1$ due to metrical specialization of the lattice are presented by Koch (1999).

3.3.8.4. *Approximate (pseudo-)coincidences of two or more lattices*

In part (iv) of Section 3.3.8.2, three-dimensional lattice coincidences and twin lattices (sublattices) were considered under two restrictions:

(*a*) the lattice coincidences (according to the twin lattice index $[j]$) are *exact* (not approximate);