Electronic Supplementary Material (ESI) for CrystEngComm.

Supplemental

Effects of grain boundary structure and shape of the solid-liquid interface on the growth direction of the grain boundaries in multicrystalline silicon

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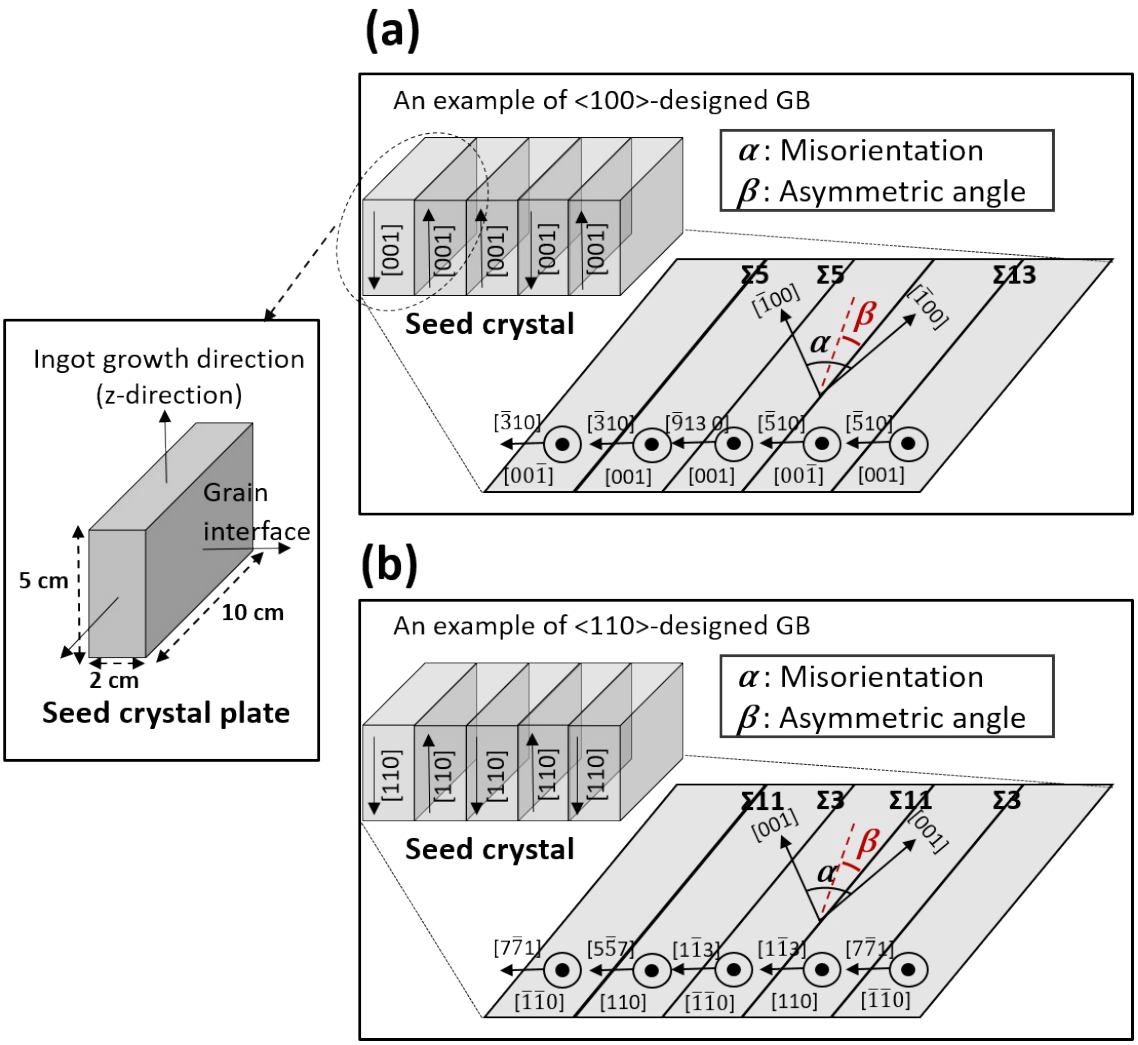


Figure S1 (a) An example of the design of the seed crystal to fabricate <100>-designed GBs. (b) An example of the design of the seed crystal to fabricate <110>-designed GBs. 4 GBs can be fabricated by combining 5 seed crystal plates.

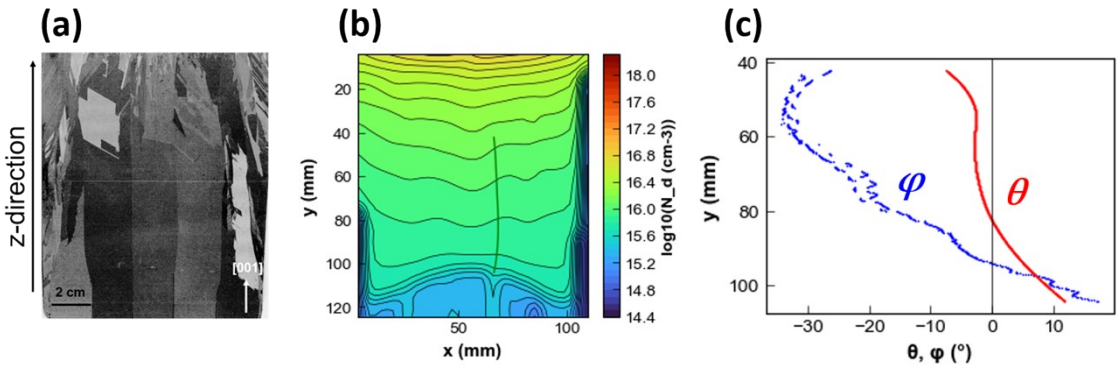
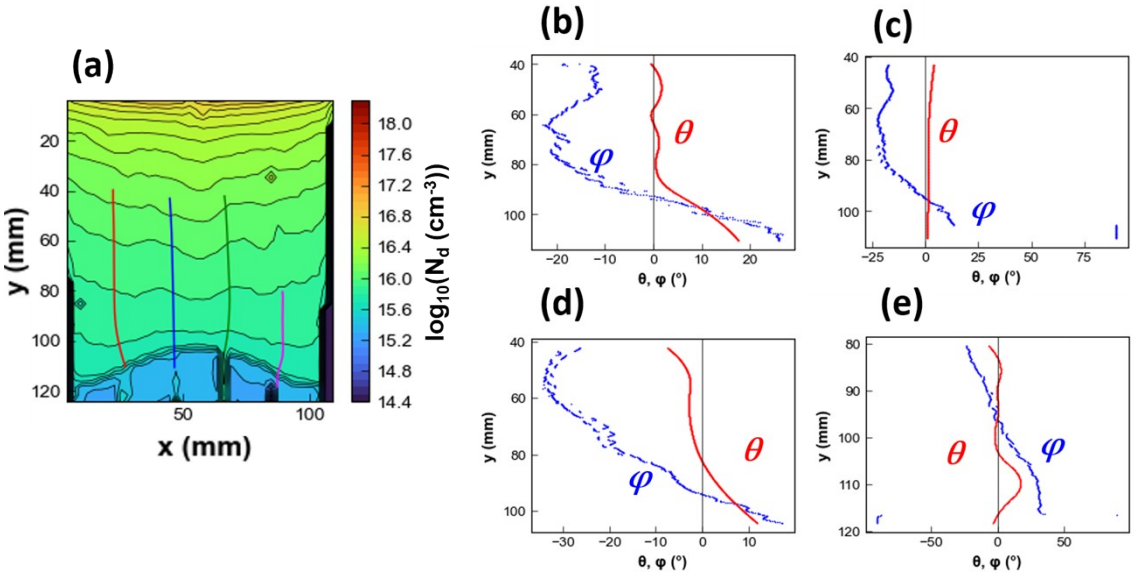


Figure S2 (a) An optical image and (b) carrier concentration of an example of the ingot cross-section with <100>-designed GBs. This distribution shows solid-liquid interface shape changes from convex to concave seen from solid with crystal growth proceeds. (c) The results of analyzing the GB plane inclination angle with respect to z-direction (θ) and the angle between the direction perpendicular to the solid-liquid interface and the z-direction (φ) for <100> (9 13 0)/($\bar{5}$10) GB (green line in Fig. S2(b))



Figures S3 (a) Carrier concentration and the position of four <100>-designed GBs. Quantitative results of θ and φ at GBs from left to right are shown in Fig. S3 (b)~(e), respectively. It is seen that the behavior of the GBs is well explained by our theory in the vicinity of the seed crystal. On the other hand, at the upper position (y = 40 ~ 80 mm), some GBs do not follow our theory as shown in Fig. S3 (b) and (c). The interaction of dislocations with GBs might be related to the phenomena. Notably, only 6 among 17 GBs showed such an unpredictable behavior, and our simple theory explains the majority of GBs.

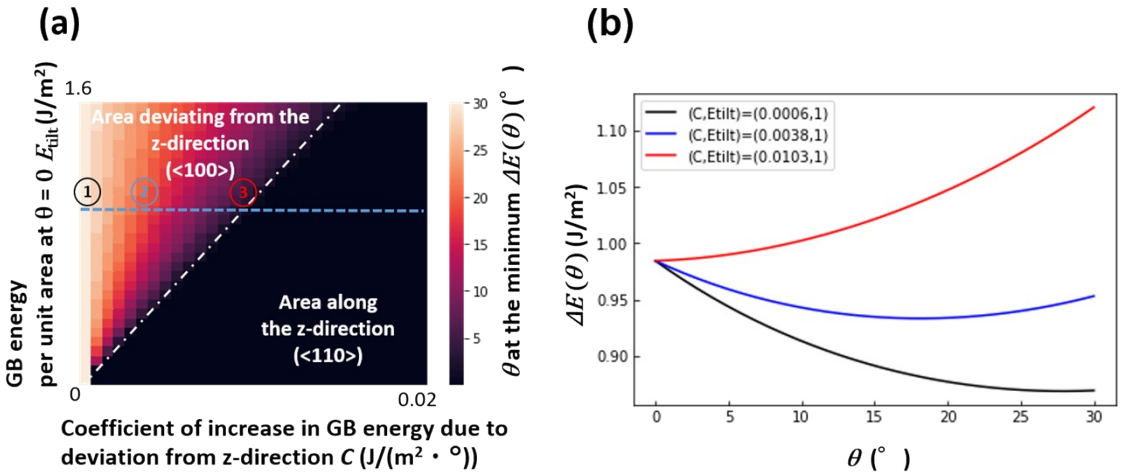


Figure S4 (a) GB growth direction θ to minimize $\Delta E(\theta)$ when $\varphi = 30°$ estimated by assuming a linear model. The GB energy per unit area (E_{tilt}) at $\theta = 0$, and the coefficient of increase of the GB energy per unit area (C) were treated as parameters (E_{tilt}: 0 ~ 1.6, C: 0 ~ 0.02,) for the calculation. (b) The relationship between $\Delta E(\theta)$ and θ at E_{tilt} and C which corresponds to 1, 2, and 3 in Figure S4(a). It is seen that the θ to minimize $\Delta E(\theta)$ varies depending on the combination of E_{tilt} and C

Table1 Relationship between GB structure, GB energy and GB growth direction.
These results suggest that the GB energies of <110>-designed GBs such as Σ3 and Σ9 GBs smaller than those of <100>-designed GBs such as Σ5, Σ13, and Σ25 GBs.

Type of GBs	E_{tilt}	Experimental behavior
{111}Σ3	0.051J/m^2 by DFT [Ref.S1]	1. θ= 0°,ϕ=7.5°(initial interface)
{221}Σ9	0.32 or 0.29 J/m^2 by DFT [Ref.S2-5]	1. θ= 0°,ϕ=8°(initial interface)
{221}Σ9	0.45 J/m^2 by molecular-dynamics simulation techniques using the Stillinger-Weber potential [Ref.S9]	1. θ= 0°,ϕ=8°(initial interface)
{310}Σ5	0.42 J/m^2 by DFT [Ref.S6-8]	1. θ= 17.6°,ϕ=28°(initial interface) 2. θ= 11.5°,ϕ=28.3°(initial interface)
{510}Σ13	0.89 J/m^2 by molecular-dynamics simulation techniques using the Stillinger-Weber potential[Ref. S9]	θ= 17.5°,ϕ=28.9°(initial interface)
{710}Σ25	0.84 J/m^2 by molecular-dynamics simulation techniques using the Stillinger-Weber potential[Ref. S9]	θ= 1.5°,ϕ=6.8°(initial interface)

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