

Supporting Information

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Sequentially PVD-Grown Indium and Gallium Selenides Under Compositional and Layer Thickness Variation: Preparation, Structural and Optical Characterization

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Supplementary

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Figure S1: Measured Raman spectra of pure In, Ga, and glass.



Figure S2: Measured Raman spectra of GaSe (prepared by chalcogenization in high Se background of a 40 nm Ga precursor film) immediately after preparation, after being exposed to air during the various measurements (rep) or for three days (Ox).

Table S1: Overview of XRD-database files from where the peak lines representing different compounds and phases of In-Se in Figure 3 were extracted.

COD: Crystallography Open Database (http://www.crystallography.net)

SD: Springer Materials (for In₄Se₃ https://materials.springer.com/isp/crystallographic/docs/sd_0451600)

	chemical formula	Data base no
150 nm, 0.2 g Se	γ-In ₂ Se ₃	COD_2106380
150 nm, 0.1 g Se	γ-In ₂ Se ₃	COD_2106380
150 nm, high Se BG	<mark>β-/γ-InSe</mark> ; In₄Se₃	COD_9008967/ COD_1534648 ; SD_0451600
150 nm, low Se BG	α -/ β -In ₂ O ₃ ; In	COD_9015718; COD_1512513
100 nm, 0.2 g Se	γ-In ₂ Se ₃	COD_2106380
100 nm, 0.1 g Se	γ-In ₂ Se ₃	COD_2106380
100 nm, high Se BG	β-/γ-InSe	COD_9008967/ COD_1534648
100 nm, low Se BG	β -/ γ -InSe ; α -/ β -In ₂ O ₃	COD_9008967/ COD_1534648 ; COD_9015718
40 nm, high Se BG	γ -In ₂ Se ₃ ; α -In ₂ Se ₃	COD_2106380 ; COD_1528775
40 nm, low Se BG	γ -In ₂ Se ₃ ; α -In ₂ Se ₃	COD_2106380 ; COD_1528775
20 nm, high Se BG	γ -In ₂ Se ₃ ; α -In ₂ Se ₃	COD_2106380 ; COD_1528775
20 nm, low Se BG	α-In ₂ Se ₃ ; γ-In ₂ Se ₃	COD_1528775; COD_2106380

Table S2: Overview of XRD-database files from where the peak lines representing different compounds and phases of Ga-Se in Figure 4 were extracted.

COD: Crystallography Open Database (http://www.crystallography.net)

ICSD: FIZ-Karlsruhe, Leibniz Institute for Information Infrastructure (http://icsd.fiz-karlsruhe.de)

	chemical formula	Data base no
150 nm, 0.2 g Se	α -/ β -Ga ₂ Se ₃	COD_2020137 / ICSD_35028
150 nm, 0.1 g Se	α-/β-Ga ₂ Se ₃	COD_2020137 / ICSD_35028
150 nm, high Se BG	β-/γ-/δ-/ε-GaSe	COD_1530863 / ICSD_73388 / COD_2106698 / COD_2105478
150 nm, low Se BG	β-Ga ₂ O ₃ ; Ga	COD_2004987; COD_8104301
100 nm, 0.2 g Se	α-/β-Ga ₂ Se ₃	COD_2020137 / ICSD_35028
100 nm, 0.1 g Se	α -/ β -Ga ₂ Se ₃	COD_2020137 / ICSD_35028
100 nm, high Se BG	β-/γ-/δ-/ε-GaSe	COD_1530863 / ICSD_73388 / COD_2106698 / COD_2105478
100 nm, low Se BG	<mark>β-Ga</mark> 2O ₃ ; β-/γ-/δ-/ε-GaSe ; Ga	COD_2004987; COD_1530863 / ICSD_73388 / COD_2106698 / COD_2105478; COD_8104301
40 nm, high Se BG	β-/γ-/δ-/ε-GaSe	COD_1530863 / ICSD_73388 / COD_2106698 / COD_2105478
40 nm, low Se BG	β-Ga ₂ O ₃ ; Ga	COD_2004987; COD_8104301
20 nm, high Se BG	α -/ β -Ga ₂ Se ₃	COD_2020137 / ICSD_35028
20 nm, low Se BG	Ga ; β-Ga ₂ O ₃	COD_8104301 ; COD_2004987



Figure S3: Tauc plot of $(\alpha E)^2$ for potential derivation of direct band gap value from linear fitting; In-Se samples with 150, 100, 40 or 20 nm In precursor thickness and selenized in various Se content (BG = background).



Figure S4: Tauc plot of $(\alpha E)^{1/2}$ for potential derivation of indirect band gap value from linear fitting; In-Se samples with 150, 100, 40 or 20 nm In precursor thickness and selenized in various Se content (BG = background).



Figure S5: Tauc plot of $(\alpha E)^2$ for potential derivation of direct band gap value from linear fitting; Ga-Se samples with 150, 100, 40 or 20 nm Ga precursor thickness and selenized in various Se content (BG = background).



Figure S6: Tauc plot of $(\alpha E)^{1/2}$ for potential derivation of indirect band gap value from linear fitting; Ga-Se samples with 150, 100, 40 or 20 nm Ga precursor thickness and selenized in various Se content (BG = background).