p-Type Doping and Alloying of CuI Thin Films with Selenium

Philipp Storm,* Michael Sebastian Bar, Susanne Selle, Holger von Wenckstern, Marius Grundmann, and Michael Lorenz

The impact of the intentional selenium doping of CuI thin films is investigated concerning crucial crystalline, electrical and optical properties. For selenium contents in between \(x(\text{Se}) = 0.1\ \text{at.}\%\) and \(x(\text{Se}) = 1\ \text{at.}\%\), the carrier density can be systematically adjusted by the selenium supply during growth between \(p = 10^{15}\ \text{cm}^{-3}\) and \(p = 8 \times 10^{17}\ \text{cm}^{-3}\) while transparency and crystallinity remain unaffected. By temperature-dependent Hall-effect measurements, a carrier freeze out is observed and the binding energy of the selenium dopant is determined. The long-term electrical stability in combination with Al\(_2\)O\(_3\) cappings is significantly improved compared to undoped or oxygen doped CuI. However, for selenium contents exceeding \(x(\text{Se}) = 1\ \text{at.}\%\), major crystalline changes are observed that are presumably correlated to a phase transformation. Transmission and electrical measurements suggest that the solubility limit of Se in CuI is about 1 at.\% since a degradation of the transparency and decreasing free hole densities are observed for Se contents exceeding 1 at.\%. Hence, the doping limit for Se in CuI corresponds to \(\approx 1\ \text{at.}\%\).

1. Introduction

To obtain transparent, complementary electronics with well investigated and unipolar n-type semiconductors such as ZnO, In\(_2\)O\(_3\), or Ga\(_2\)O\(_3\), a similarly transparent semiconducting p-type material is required. As a promising candidate, copper iodide (CuI) emerged, unifying a high transparency up to 90% in the visible range, a wide bandgap energy of \(E_g = 3.1\ \text{eV}\) and excellent hole transport properties (hole mobilities up to \(\mu = 44\ \text{cm}^2\ \text{V}^{-1}\ \text{s}^{-1}\) and carrier densities up to \(p = 10^{20}\ \text{cm}^{-3}\)[1–4]) The high excitonic binding energy of \(E^0_b = 58\ \text{meV}\) also favors potential applications in optoelectronics.[5] At standard environmental conditions, the zinc-blende \(\gamma\)-phase is the thermodynamically stable crystal structure. However, a complex phase diagram exists at higher pressures and temperatures.[6,7]

Thin film growth has already been demonstrated by various methods such as spin coating,[8] iodization,[9,10] thermal evaporation,[11] sputtering,[12] ion beam sputtering,[13] molecular beam epitaxy,[14] or pulsed laser deposition (PLD).[15] The high and usually degenerate conductivity of CuI is often attributed to intrinsic copper vacancies.[1,16–18] However, doping attempts with iodine, exploiting the intrinsic defects, are inconclusive and seemingly dependent on the growth technique.[19–21] Recent results of PLD grown CuI capped with amorphous Al\(_2\)O\(_3\) suggest an extrinsic influence on the electrical properties.[22] In particular, the incorporation of oxygen acceptors in combination with diffusion through the Al\(_2\)O\(_3\) capping dominates the conductivity. However, since the oxygen concentration and therefore also the carrier density depend on external conditions, oxygen is no suitable dopant toward stable electrical properties. To resolve these issues, we report on selenium as acceptor dopant and evaluate its impact on the crystalline, electrical, as well as optical properties of CuI thin films.

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2. Experimental Results

CuI:Se thin films were grown on c-sapphire substrates at a constant growth temperature of \(T_g \approx 140^\circ\text{C}\) and growth pressure of \(p(N_2) = 3 \times 10^{-3}\ \text{mbar}\). The selenium content of the PLD plasma was systematically varied utilizing elliptically segmented vertical continuous composition spread (VCCS) targets. For more information concerning the VCCS-growth technique, refer to the studies by Kneiß et al. and von Wenckstern and co-workers[23,24] The given Se contents of the thin films represent the time-averaged Se content within the PLD plasma as

* Corresponding author.

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calculated by Monte Carlo simulations presented in ref. [24]. The selenium content is always relative to the iodine composition. For more information on crucial thin film properties of PLD-grown CuI and the effect of Al₂O₃ capping layers, please refer to the studies by Storm and co-workers[15,22]. Wide-angle X-ray diffraction (XRD) 2θ-ω scans of binary CuI and doped CuI:Se thin films on c-sapphire are shown in Figure 1a. For all samples, the CuI grows exclusively in (111) orientation up to the highest investigated selenium content of x(Se) = 10 at.%. However, in the magnified view on the CuI(111) and CuI(333) reflections, shown in Figure 1b, more than just one CuK₀₁ thin film reflection is observed for Se contents exceeding 1 at.%. The reflection located at the low-angle side is designated R2 and the reflection on the high-angle side is designated R1. Compared to a binary CuI thin film, it is apparent that R1 belongs to the expected γ-CuI reflections. For the unknown reflection R2, the relative intensity compared to R1 increases with increasing selenium contents and is the only one remaining for the highest investigated x(Se) = 10 at.%. In general, the calculated out-of-plane lattice constant (assuming a cubic symmetry) of R2 is significantly higher compared to γ-CuI. The lattice constants were determined utilizing all CuI(nnn) reflections of R1 or R2, goniometer-error extrapolation, and correction of sample miss-alignment with α-Al₂O₃ literature values (JCPDS 82-1399), the peak positions of R1 and R2 shift to the higher angles, i.e., lower lattice constants according to

$$a_{R1}^{αI}(Å) = (6.061 ± 0.002) - (0.0012 ± 0.0008) \times x(Se)$$  \hspace{1cm} (1)

$$a_{R2}^{αI}(Å) = (6.086 ± 0.008) - (0.0007 ± 0.0001) \times x(Se)$$  \hspace{1cm} (2)

as shown in the inset of Figure 1b. This is within expectation regarding the smaller ionic radius of selenium (r₁,Se = 198 pm) compared to iodine (r₁,Ι = 220 pm) [25] and verifies the incorporation of selenium on the iodine site in both, R1 and R2. Therefore, it is also not expected that the R2 reflections with their larger assigned lattice constants originate from selenium-rich γ-CuI. Instead, R2 can probably be caused by another environmentally stable crystal structure of CuI that is stabilized or catalyzed by the selenium during thin film growth. The general crystallinity, expressed by the 2θ full width at half maximum (FWHM), of R1 features FWHM values for the (111) reflection of \( Δθ_{(111)} \approx (0.07 ± 0.01)^{°} \) independent of the selenium content and corresponding peak shift. For R2, however, \( Δθ_{(111)} \) increases with increasing selenium content from \( Δθ_{(111)} = 0.092^{°} \) at \( x(Se) = 1 \) at.% to \( Δθ_{(111)} = 0.154^{°} \) at \( x(Se) = 10 \) at.%, despite the increasing intensity of the R2 reflection with increasing selenium contents. Therefore, the increasing incorporation of selenium has detrimental effects on the crystalline quality of the parts of the thin films causing the R2 reflections whereas the γ-CuI(nnn) R1 reflections remain unaffected.

To evaluate the impact of selenium incorporation on the electrical properties of CuI thin films, Hall-effect measurements were conducted. The Hall samples were grown on EagleXG glass substrates and capped with 30 nm Al₂O₃ grown in nitrogen at p(N₂) = 3 \times 10⁻³ mbar. The carrier densities for corresponding thin films are shown in Figure 2a. In general, no significant differences between Hall-effect measurements of 1 μm or 250 nm thick CuI:Se films are observed, confirming the measurement of “bulk”-like properties of the films and not that of thin surface or interface layers. For low selenium contents \( x(Se) < 1 \) at.% with only negligible consequences on the crystalline quality, the carrier density increases from \( p \approx 10^{15} \) cm⁻³ at \( x(Se) = 0.2 \) at.% to \( p = 8 \times 10^{17} \) cm⁻³ at \( x(Se) = 1 \) at.%. At \( x(Se) = 1 \) at.%, the carrier density reaches a maximum and decreases for further increasing selenium contents down to \( p = 10^{16} \) cm⁻³ at \( x(Se) = 4 \) at.%. If \( x(Se) \) is increased even further, the carrier density increases again to \( p = 8 \times 10^{16} \) cm⁻³ at \( x(Se) = 10 \) at.%, which also represents the highest investigated selenium content. In general, the evolution of the electrical properties seems to be correlated to the crystalline properties of the thin film. Although the doping regime below \( x(Se) = 1 \) at.% is

![Figure 1](image-url). a) Wide-angle XRD 2θ-ω scans for various selenium contents for uncapped 1 μm CuI:Se and 250 nm binary CuI thin films on c-sapphire. The thin films were grown at \( T_g = 140^{°}C \) and p(N₂) = 3 \times 10⁻³ mbar. b) Zoomed-in view on the CuI(111) and CuI(333) reflections with the two separate reflections designated by R1 and R2. Additional reflections caused by CuK₀₁, CuK₀₂, and W₁₆ radiation are designated correspondingly. The inset shows the evolution of the calculated out-of-plane lattice constant \( a_{l} \) in dependence of the selenium content x(Se) for a cubic symmetry for R1 (green) and R2 (black). The 2θ-FWHM and peak positions of the reflections were determined by deconvolution of the CuK₀₁/CuK₀₂ reflections of R1 and R2, respectively.
characterized by increasing carrier densities with increasing selenium content, the appearance of the R2 reflection at \( x(\text{Se}) = 1 \text{ at.\%} \) coincides with the carrier density maximum that is also observed close to \( x(\text{Se}) = 1 \text{ at.\%} \). In the investigated alloy regime between \( x(\text{Se}) = 1 \text{ at.\%} \) and \( x(\text{Se}) = 10 \text{ at.\%} \), the transition from dominantly R1 to solely R2 takes place. In this picture, the decreasing carrier densities slightly above \( x(\text{Se}) = 1 \text{ at.\%} \) can be caused by replacement of higher conductive R1 \( \gamma \)-CuI:Se in the crystal by less conductive R2. Since R2 is still continuously doped by selenium, the carrier density increases again for increasing \( x(\text{Se}) \).

Concerning the corresponding Hall-effect mobilities, no systematic trend in dependence of the selenium content as shown in Figure 2b is observed. The measured hole mobilities vary over one order of magnitude from \( 2.5 \text{ cm}^2\text{V}^{-1}\text{s}^{-1} \) at \( x(\text{Se}) = 10 \text{ at.\%} \) to \( 21 \text{ cm}^2\text{V}^{-1}\text{s}^{-1} \) at \( x(\text{Se}) = 1 \text{ at.\%} \). However, since most investigated samples were grown at around \( x(\text{Se}) = 1 \text{ at.\%} \) and are quite dispersed concerning their Hall-effect mobilities, they were also statistically sorted as shown in the inset of Figure 2b. The highest count number is obtained for the interval \( \mu = [7.5, 12.5] \text{ cm}^2\text{V}^{-1}\text{s}^{-1} \) with decreasing counts for higher or lower mobilities. The corresponding mean mobility in this doping range is \( \approx 10.3 \text{ cm}^2\text{V}^{-1}\text{s}^{-1} \) with a standard deviation of 5.7 cm²V⁻¹s⁻¹.

To determine the activation energy of the selenium dopant in CuI:Se, temperature-dependent Hall-effect measurements were conducted on samples with moderate doping. As shown in Figure 2c for samples with \( x(\text{Se}) \approx 1 \text{ at.\%} \) doping, the carrier density decreases with decreasing temperature. For the highest doped sample, a slope change attributed to compensation is observed at \( \tilde{\mu} = N_D = (6 \pm 5) \times 10^{14} \text{ cm}^{-3} \). Unfortunately, no such features were observed for lower doped samples. Therefore, the activation energies were evaluated for both cases (uncompensated or compensated) with \( E_{A,\text{comp}} = E_{A,\text{uncomp}}/2 \).

![Figure 2](https://www.advancedsciencenews.com)
The activation energy and acceptor density was determined by fitting the compensated single-acceptor Boltzmann approximation for \( p \):[26]

\[
p = \frac{1}{2g}N_v \exp\left( -\frac{E_A}{k_BT} \right) \left[ \sqrt{\alpha^2 + 4\hat{g}^2 \frac{N_A - N_D}{N_v} \exp\left( \frac{E_A}{k_BT} \right)} - \alpha \right]
\]

with \( \hat{g} = 1 \) (assumption since corresponding literature for the selenium acceptor is missing to the best of the authors knowledge), \( m_{\text{eff}} = 0.3 \times m_e \) [1] and valence band density of states with respect to the quadratic band approximation

\[
N_v = 2\left( \frac{m_{\text{eff}} k_B T}{2\pi \hbar^2} \right)^{3/2}
\]

as well as

\[
\alpha = 1 + \hat{g} \frac{N_D}{N_v} \exp\left( \frac{E_A}{k_BT} \right).
\]

For samples without features attributable to compensation in the temperature-dependent Hall-measurements (data shown in blue and violet in Figure 2c), the uncompensated solution with \( \alpha = 1 \) and \( N_D = 0 \) cm\(^{-3}\) was utilized. Fitting the model yields the activation energy in dependence of the acceptor concentration as shown in the inset of Figure 2c. The resulting binding energy \( E_b \) was determined by fitting of the dependence:[26]

\[
E_A = E_b - \beta N_A^{3/2}.
\]

The corresponding activation energies for the uncompensated case (blue line in the inset of Figure 2c) yield a high acceptor binding energy of \( E_{b,\text{uncomp}} = (240 \pm 5) \) meV. However, since only 98% purity powders of Cul were used in the powder targets, it is also reasonable to assume that the Cul is compensated for lower acceptor concentrations even though typical features were not directly observed. The corresponding binding energy for the compensated case is \( E_{b,\text{comp}} = (78 \pm 23) \) meV (red line in the inset of Figure 2c). Compared to density functional calculations,[23] a charge transition level for selenium at 265 meV was calculated, close to our experimental binding energy for the uncompensated case. In general, the determined acceptor concentrations of \( N_A \approx 10^{16} \) cm\(^{-3}\) are significantly lower than expected for \( x(\text{Se}) \approx 1 \) at.\% yielding \( N_A \approx 10^{20} \) cm\(^{-3}\). Therefore, either selenium is excessively desorbed during growth or is incorporated/coordinated in a way such that only a fraction is actually acting as an electrically contributing acceptor.

To also evaluate the potential of selenium-doped Cul regarding its electrical stability in combination with an \( \text{Al}_2\text{O}_3 \) capping grown in nitrogen, corresponding 120 nm Cul:Se thin films with a 30 nm \( \text{Al}_2\text{O}_3 \) capping were measured over multiple hours as shown in Figure 2d. For these sample parameters, very strong increase in the resistivity (up to four orders of magnitude) as a consequence of decreasing carrier densities was observed for undoped or oxygen-doped Cul.[22] This behavior is contributed to the diffusion of oxygen between Cul and the \( \text{Al}_2\text{O}_3 \). However, as shown in Figure 2d, the electrical resistivity for various Cul:Se samples grown at different growth temperatures \( T_1 \) changes only little over time with maximum–minimum ratios of 1.2 to 1.08 after 20 h. In addition to a small resistivity increase shortly after growth, these variations are mostly caused by slightly decreasing resistivities as a consequence of the thin and insufficient capping. Therefore, the selenium is not seemingly affected by the same diffusion process that occurs for oxygen and therefore results in much more stable electrical properties. In general, a trend to higher resistivities with increasing growth temperatures is observed, similar to previous investigations of PLD-grown Cul.[15] However, the usually applied \( \text{Al}_2\text{O}_3 \) capping is still far from being sufficient, in particular concerning the long-term oxygen shielding toward consistent carrier densities on a year’s scale. Therefore, SiN\(_x\)O\(_y\) was investigated as another capping material that can be grown by PLD in situ. A corresponding time-dependent measurement of the resistivity of 120 nm Cul capped with \( \approx 10 \) nm SiN\(_x\)O\(_y\) is shown in Figure 2d. Initially, no resistivity increase is observed and the measured resistivities align closely to the device limit. After merely \( \approx 3 \) h, the resistivities start to decrease rapidly and saturate after \( \approx 1 \) week at \( \rho \approx 1 \) \( \Omega \cdot \text{cm} \). Therefore, solely SiN\(_x\)O\(_y\) is not suited as a long-term stable capping material. However, to resolve these issues, a heterostructure capping approach was investigated. Utilizing \( \text{Al}_2\text{O}_3 \) (grown in N\(_2\)/SiN\(_x\)O\(_y\) superlattices, a reduction or suppression of the oxygen diffusion is targeted by increased oxygen trapping in the SiN\(_x\)O\(_y\) layers compared to \( \text{Al}_2\text{O}_3 \) and multiple heterointerfaces acting as diffusion barriers. As shown in Figure 2d for 120 nm Cul, even after 4 weeks, the resistivity is still very high at \( \rho \approx 4 \times 10^4 \) \( \Omega \cdot \text{cm} \) and shows no signs of degradations in terms of changes of resistivity. This renders corresponding superlattice cappings a promising approach, even though more investigations on thermal, light-induced, moist, and long-term stress are necessary.

Since the incorporation of selenium results in major crystal changes in the alloy regime, transmission measurements were conducted to evaluate their impact on the optical properties as shown in Figure 3a. For \( x(\text{Se}) = 1 \) at.\%, the transmittance spectrum is very similar to binary Cul grown by PLD as reported.[15] Thickness interference dominates below the band edge with an average transmittance of \( \approx 80\% \). Pronounced excitonic absorption is visible at \( E_{\text{Tauc}}/Z_1 = (3.05 \pm 0.01) \) eV and the corresponding transition due to spin–orbit coupling at \( E_{\text{z}} = (3.68 \pm 0.01) \) eV. As soon as the selenium content is increased to \( x(\text{Se}) = 4 \) at.\%, characteristic features in the spectra broaden or even vanish. The excitonic transitions \( Z_1/Z_2 \) and \( Z_3 \) are much less pronounced and their width increases. The energetic position of \( Z_1/Z_2 \) also shifts slightly to higher energies at \( E_{Z_1/Z_2} = (3.07 \pm 0.01) \) eV. For a selenium content of \( x(\text{Se}) = 7 \) at.\%, no features of excitonic absorption are visible at all. However, for \( x(\text{Se}) = 10 \) at.\%, a dip below the expected energy at \( E_\text{v} = (2.98 \pm 0.02) \) eV can be attributed to excitonic absorption, possibly originating from R2. As shown in Figure 3b, the absorbance below the bandgap energy is generally increased with increasing selenium contents. Although no significant changes compared to binary Cul below \( x(\text{Se}) < 4 \) at.\% are observed, higher selenium contents result in decreasing Tauc bandgaps to \( E_{\text{Tauc}} = (2.75 \pm 0.05) \) eV for \( x(\text{Se}) = 7 \) at.\% and \( E_{\text{Tauc}} = (2.58 \pm 0.09) \) eV for \( x(\text{Se}) = 10 \) at.\%.
3. Conclusion

The impact of selenium on the crystalline, electrical, and optical properties of CuI was investigated. Concerning the crystallinity of corresponding thin films, unidentified XRD reflections close to the γ-CuI reflection appeared and successively replaced the γ-CuI reflection if the selenium content was increased to x(Se) = 1 at.% and higher. We explored the doping limits of intentional p-doping in a range between p = 10^{15} cm^{-3} at x(Se) = 0.2 at.% and p = 8 \times 10^{17} cm^{-3} at x(Se) = 1 at.%.

Further increases in x(Se) result in decreasing carrier densities, presumably correlated to the simultaneously occurring crystalline changes. The hole mobilities across the investigated alloy range vary strongly between 2.5 cm^{2}V^{-1}s^{-1} at x(Se) = 10 at.% and 21 cm^{2}V^{-1}s^{-1} at x(Se) = 1 at.%.

The binding energy of the selenium dopant was determined by temperature-dependent Hall-effect measurements assuming compensated (E_{\text{H,comp}} = (78 \pm 23) meV) or uncompensated (E_{\text{H,uncomp}} = (240 \pm 5) meV) CuI. The long-term behavior was studied by time-dependent resistivity measurements and revealed significantly more stable properties compared to undoped or intentionally oxygen-doped CuI for Al_{2}O_{3} capping grown in N_{2}. As a promising oxygen barrier, Al_{2}O_{3}/SiN_{x}O_{y} superlattice cappings were investigated that prevent any notable resistivity decreases close to a month-scale and presumably even much longer. The optical properties were evaluated by transmission measurements. Up to x(Se) = 1 at.%, the spectra are identical to undoped, binary CuI with a high average transparency in the visible range of ~80%. However, for x(Se) > 1 at.%, the excitonic absorption starts to vanish and absorption below the bandgap energy of binary CuI appears.

Since weakly doped CuI:Se x(Se) < 1 at.% exhibits a significantly increased stability of crucial electrical properties, undoubtedly bulk conductivity, and widely modifiable carrier densities in combination with a suitable capping, it is a promising material for various device applications such as thin film transistors or diodes.

4. Experimental Section

The thin films were grown by PLD utilizing powder-based targets. For all CuI targets, corresponding powders were pressed into steel or copper forms and sintered at room temperature (RT). The surface of the target was molten during initial conditioning with at least 5,000 laser pulses at RT. We used binary, homogeneous CuI (Cu: Carl Roth 98%) targets and elliptically segmented (VCCS) CuI+10at.%CuSe/CuI+1at.%CuSe and CuI+1at.%CuSe/CuI targets (CuSe: 99.95% Alfa Aesar). To produce the Al_{2}O_{3} targets, Al_{2}O_{3} powders (Alfa Aesar 99.999%) were pressed and sintered at 1650 °C for 6 h. The SiN_{x}O_{y} thin films were grown utilizing single-crystalline Si crystals. The PLD system consisted of a Coherent LPX Pro 305 248 nm KrF excimer laser operating at a pulse energy of 650 mJ. The samples were grown with a laser pulse frequency of 10 Hz. The Al_{2}O_{3} capping and CuI thin films were grown in a nitrogen atmosphere. The SiN_{x}O_{y} depositions were conducted in p(N_{2}) = 3 \times 10^{-3} mbar atmosphere. The SiN_{x}O_{y} depositions were conducted in p(N_{2}) = 3 \times 10^{-3} mbar or p(N_{2}) = 9 \times 10^{-5} mbar. The thin films were grown at an indicated growth temperature of T_{\text{g}} = 140°C if not explicitly stated otherwise. The growth temperature of the Al_{2}O_{3} capping was similar to the preceding CuI thin film. C-sapphire and EagleXG substrates were utilized. X-ray diffraction 2\theta-\omega measurements were performed with a PANalytical X’Pert PRO materials research diffractometer equipped with a Cu K_{x} radiation source, parabolic mirror, and PIlXcel detector. Transmission measurements were conducted utilizing a PerkinElmer Lambda 19 spectrometer at RT. The electronic properties were measured with a home-built four-probe van der Pauw technique Hall-effect measurement setup operating at 0.43, 0.75, and 1.1 T or a Quantum Design Physical Property Measurement System at 9 T. DC-sputtered gold was used for the electrical contacts. The thickness of the CuI and Al_{2}O_{3} layers was estimated on growth rates we previously presented.[15] The growth rate of the SiN_{x}O_{y} was determined by a separate deposition on c-sapphire and estimation of the thickness with a Bruker Dektak XT profilometer.

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Conflict of Interest
The authors declare no conflict of interest.

Data Availability Statement
The data that support the findings of this study are available from the corresponding author upon reasonable request.

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