

# Bibliography

- [1] W. Fuhs and R. Klenk. *Advances in Solar Energy*, chapter Thin-Film Solar Cells, page 409. American Solar Energy Society, 1999.
- [2] R.W. Birkmire. Compound polycrystalline solar cells: Recent progress and Y2K perspective. *Solar Energy Materials and Solar Cells*, 65:17–28, 2001.
- [3] M. A. Contreras, B. Egaas, K. Ramanathan, J. Hiltner, A. Schwartzlander, F. Hasoon, and R. Noufi. Progress towards 20 % efficiency in Cu(In,Ga)Se<sub>2</sub> polycrystalline thin-film solar cells. *Progr. Photovolt.: Res. Appl.*, 7(4):311–316, 1999.
- [4] U. Rau and H. W. Schock. Electronic properties of Cu(In,Ga)Se<sub>2</sub> heterojunction solar cells -recent achievements, current understanding, and future challenges. *Appl. Phys. A*, 1999.
- [5] C. Heske, D. Eich, R. Fink, E. Umbach, T. van Buuren, C. Bostedt, L. J. Terminello, S. Kakar, M. M. Grush, T. A. Callcott, F. J. Himpsel, D. L. ederer, R. C. C. Perera, W. Riedl, and F. Karg. Observation of the intermixing at the buried CdS/Cu(In,Ga)Se<sub>2</sub> thin film solar cell heterojunction. *Appl. Phys. Lett.*, 74:1451–1453, march 1999.
- [6] U. Rau, M. Schmitt, F. Engelhardt, Th. Meyer, O. Seifert, J. Parisi, W. Riedl, and F. Karg. Defect spectroscopy and electrical transport in Cu(In,Ga)Se<sub>2</sub> solar cells. In *Proc. of 14<sup>th</sup> EPVSC*, 1997.
- [7] R. Klenk. Characterisation and modelling of chalcopyrite solar cells. *Thin Solid Films*, 387:135–140, 2001.
- [8] J. E. Jaffe and A. Zunger. Electronic structure of the ternary chalcopyrite semiconductors CuAlS<sub>2</sub>, CuGaS<sub>2</sub>, CuInS<sub>2</sub>, CuAlSe<sub>2</sub>, CuGaSe<sub>2</sub>, and CuInSe<sub>2</sub>. *Phys. Rev. B*, 28:5822–5847, 1983.
- [9] J. E. Jaffe and A. Zunger. Theory of the band-gap anomaly in ABC<sub>2</sub> chalcopyrite semiconductors. *prb*, 29:1882–1906, 1984.
- [10] R. Klenk, P. Dobson, M. Falz, N. Janke, J. Klaer, I. Luck, A. Pérez-Rodríguez, R. Scheer, and E. Terzini. SULFURCELL: Efficient Thin Film Solar Cells Based on CuInS<sub>2</sub>. In *Proceedings of 16th EPVSEC, Glasgow*, 2000.
- [11] K. Siemer, J. Klaer, I. Luck, J. Bruns, R. Klenk, and D. Bräunig. Efficient CuInS<sub>2</sub> solar cells from a rapid thermal process (RTP). *Solar Energy Materials and Solar Cells*, 67:159–166, 2001.
- [12] U. Blieske, V. Dieterle, I. Hengel, Ch. Kaufmann, R. Klenk, and M. Ch. Lux-Steiner. Loss-analysis and modification of CuInS<sub>2</sub> based solar cells. In *Proc. 14<sup>th</sup> EPVSEC*, pages 2135–2138, 1997.
- [13] I. Hengel, A. Neisser, R. Klenk, and M. Ch. Lux-Steiner. Current transport in CuInS<sub>2</sub>:Ga/CdS/ZnO -solar cells. *Thin Solid Films*, 361–362:458–462, 2000.
- [14] T. Watanabe and M. Matsui. Improved Efficiency of CuInS<sub>2</sub>-Based Solar Cells without Potassium Cyanide Process. *Jap. J. Appl. Phys.*, 38:L1379–L1381, 1999.
- [15] H. Hahn, G. Frank, W. Klinger, A.-D. Meyer, and G. Störger. Über einige ternäre Chalkogenide mit Chalcopyritstruktur. *Z. anorg. allg. Chemie*, 271:153–170, 1953.
- [16] S. Wagner, J. L. Shay, B. Tell, and H. M. Kasper. Green electroluminescence from CdS-CuGaS<sub>2</sub> heterodiodes. *Appl. Phys. Lett.*, 22(8):351–353, 1973.

- [17] R.C. Smith. Device applications of the ternary semiconducting compounds. *Journal de Physique*, Colloque C3, supplément au n<sup>o</sup> 9, Tome 36:C3-89-C3-99, 1975.
- [18] S. Wagner, J.L. Shay, and H.M. Kasper. The p-CuInSe<sub>2</sub>/n-CdS heterodiode: photovoltaic detector, solar cell and light emitting diode. *Journal de Physique*, Colloque C3, supplément au n<sup>o</sup> 9, Tome 36:C3-101-C3-104, 1975.
- [19] P. M. Bridenbaugh and P. Migliorato. Junction electroluminescence in CuInS<sub>2</sub>. *Appl. Phys. Lett.*, 26(8):459-460, 1975.
- [20] J.L. Shay and J.H. Wernik. *Ternary Chalcopyrite Semiconductors: Growth, Electronic Properties and Applications*. Pergamon Press, Oxford, 1975.
- [21] B. R. Pamplin. Non-Stoichiometry and Solid Solutions in Adamantine Ternary Compounds. *Journal de Physique*, Colloque C3, supplément au n<sup>o</sup> 9, Tome 36:C3-53-C-56, 1975.
- [22] B.R. Pamplin. Ternary Chalcopyrite Compounds. *Progress in Crystal Growth Charact.*, 1:331-387, 1979.
- [23] S. C. Abrahams and J. L. Bernstein. Piezoelectric nonlinear optic CuGaS<sub>2</sub> and CuInS<sub>2</sub> crystal structure: Sublattice distortion in A<sup>I</sup>B<sup>I</sup>IIC<sub>2</sub><sup>V</sup>I and A<sup>I</sup>IB<sup>I</sup>VC<sub>2</sub><sup>V</sup> type chalcopyrites. *J. Chem. Phys.*, 59:5415-5422, 1973.
- [24] H. W. Spiess, U. Haeberlen, G. Brandt, A. Räuber, and J. Scheider. Nuclear Magnetic Resonance in I<sub>B</sub>-III-VI<sub>2</sub> Semiconductors. *Phys. Stat. Sol. (b)*, 62:183-192, 1974.
- [25] N. Yamamoto and T. Miyauchi. Growth of Single Crystals of CuGaS<sub>2</sub> and CuGa<sub>(1-x)</sub>In<sub>x</sub>S<sub>2</sub> in In Solution. *Jap. J. Appl. Phys.*, 11:1383-1384, 1972.
- [26] T. Miyauchi, N. Yamamoto, Y. Hamakawa, and T. Nishino. Composition Dependence of Band Gaps of CuGa<sub>1-x</sub>In<sub>x</sub>S<sub>2</sub>. *Jap. J. Appl. Phys.*, 12:606-607, 1973.
- [27] I.V. Bodnar. Growth and Properties of Solid Solutions CuGa<sub>x</sub>In<sub>1-x</sub>S<sub>2</sub>. *Inorganic Materials*, 17:378-382, 1981.
- [28] I.V. Bodnar and A.I. Lukomskii. The Concentration Dependence of the Band Gap for CuGa<sub>x</sub>In<sub>1-x</sub>S<sub>2</sub> and AgGa<sub>x</sub>In<sub>1-x</sub>S<sub>2</sub> Solid Solutions. *Phys. Stat. Sol. (a)*, 98:K165, 1986.
- [29] H. Miyake and K. Sugiyama. Phase diagram of the CuGaS<sub>2</sub>-In pseudobinary system. *Jap. J. Appl. Phys.*, 29:L998-L1000, 1990.
- [30] T. Kato, T. Kiuchi, T. Matsumoto, and Y. Nabetani. Growth of Cu-(Ga,In)-S system using temperature difference method under controlled S vapor pressure. In *Proc. of ICTMC-11, Salford*, pages 15-18, 1997.
- [31] L. Vegard. Die Konstitution der Mischkristalle und die Raumfüllung der Atome. *Zeitschrift für Physik*, 5(1):17-26, 1921. in German.
- [32] J.A. Groenink and P.H.Janse. A Generalized Approach to the Defekt Chemistry of Ternary Compounds. *Zeitschrift für Physikalische Chemie Neue Folge*, 110:17-28, 1978.
- [33] J.J.M. Binsma. *Crystal growth and defect chemistry of CuInS<sub>2</sub>*. PhD thesis, Katholieke Universiteit te Nijmegen, 1981.
- [34] D. C. Look and J. C. Manthuruthil. Electron and hole conductivity in CuInS<sub>2</sub>. *J. Phys. Chem. Solids*, 37:173-180, 1976.
- [35] R. Klenk, T. Walter, H. W. Schock, and D. Cahen. Physical vapour deposition of CuInX<sub>2</sub> (X=S,Se) thin films- a model for the growth mechanism. In *Proc. of POLYSE, Saint Malo*, 1993.

- 
- [36] T. Walter. *Herstellung und optoelektronische Charakterisierung polykristalliner I-III-VI<sub>2</sub> Verbindungshalbleiter und darauf basierender Heteroübergänge für Dünnschichtsolarzellen*. PhD thesis, Universität Stuttgart, 1994.
- [37] D. Braunger, S. Zweigart, and H.W. Schock. The influence of Na and Ga on the incorporation of the chalcogen in polycrystalline Cu(In,Ga)(S,Se)<sub>2</sub> thin-films for photovoltaic applications. In *Proceedings of 2nd WPVSEC, Vienna*, 1998.
- [38] R. Klenk. *Polykristalline CuGaSe<sub>2</sub>-Dünnschichten für die Photovoltaik. Herstellung und Charakterisierung von Absorbern und Heteroübergängen*. PhD thesis, Universität Stuttgart, 1993.
- [39] J. L. Shay, B. Tell, H. M. Kasper, and L. M. Schiavone. p-d-Hybridization of valence bands of I-III-VI<sub>2</sub> compounds. *Phys. Rev. B*, 3(12):5003–5005, 1972.
- [40] J.L. Shay. Experimental Studies of Energy Band Structure of Chalcopyrite Crystals. *Journal de Physique, Colloque C3, supplément au no 9*, 36:C3–109, 1975.
- [41] B. Tell, J. L. Shay, H. M. Kaspers, and R. L. Barns. Valence-band structure of CuGa<sub>x</sub>In<sub>1-x</sub>S<sub>2</sub> alloys. *Phys. Rev. B*, 10:1748–1750, 1974.
- [42] S. Shirakata, A. Ogawa, S. Isomura, and T. Kariya. Photoluminescence and Photorefectance of CuGa(S<sub>1-x</sub>Se<sub>x</sub>) and Cu(Ga<sub>1-x</sub>In<sub>x</sub>)S<sub>2</sub> Alloys. *Jap. J. Appl. Phys.*, 32 Suppl. 32-3:94–96, 1993.
- [43] T. Ohashi, M. Wakamori, Y. Hashimoto, and K. Ito. Cu(In<sub>1-x</sub>Ga<sub>x</sub>)S<sub>2</sub> thin films prepared by sulfurization of precursors consisting of metallic and gallium sulfide layers. *Jap. J. Appl. Phys.*, 37:6530–6534, 1998.
- [44] W. Shockley. The theory of p-n-junctions in semiconductors and p-n junction transistors. *Bell System Technical Journal*, pages 435–489, 1949.
- [45] I. Hengel. *Ladungsträgertransport und Rekombinationsmechanismen in Chalcopyrit-Dünnschichtsolarzellen*. PhD thesis, Fachbereich Physik, Freie Universität Berlin, Germany, 2000.
- [46] J. Reiss. private communications.
- [47] R. Herberholz, V. Nadenau, U. Rühle, C. Köble, H. W. Schock, and B. Dimmler. Prospects of wide-gap chalcopyrites for thin film photovoltaic modules. *Solar Energy Materials and Solar Cells*, 49:227–237, 1997.
- [48] S. H. Wei and A. Zunger. Band offsets and optical bowings of chalcopyrites and Zn-based II-VI alloys. *J. Appl. Phys.*, 78:3846–3856, 1995.
- [49] A. Zunger and S. H. Wei. Electronic structure theory of chalcopyrite alloys, interfaces and ordered vacancy compounds. In *Proc. 13<sup>th</sup> NREL PV program review AIP CONF Proc 353*, pages 155–160, 1996.
- [50] H. W. Schock, U. Rau, T. Dullweber, G. Hanna, M. Balboul, T. Margorian-Friedlmeier, A. Jasenek, I. Kötschau, H. Kerber, and H. Wiesner. High efficiency, high voltage solar cells by band gap and defect engineering in Cu(In,Ga)(S,Se)<sub>2</sub> chalcopyrite semiconductors. In *Proceedings of 16th EPVSEC, Glasgow*, 2000.
- [51] W.W. Gärtner. *Phys. Rev.*, 116:84, 1959.
- [52] S. M. Sze. *Physics of Semiconductor Devices*. John Wiley & Sons, New York, 2 edition, 1981.
- [53] R. Klenk and H.W. Schock. Photocurrent collection in thin film solar cells - calculation and characterization for CuGaSe<sub>2</sub>/(Zn,Cd)S. In *Proceedings of 12th EPVSEC, Amsterdam*, 2000.
- [54] J.E. Phillips. Determination of diffusion length with bi-facial spectral response. In *Proc. of IEEE PVSC*, 1990.

- [55] Ibach and Lueth. *Solid States Physisc*. Springer Verlag, 1995.
- [56] H. Neumann, W. Hörig, V. Savelev, J. Lagzdonis, B. Schumann, and G. Kühn. The optical properties of  $\text{CuInS}_2$  thin films. *Thin Solid Films*, 79:167–171, 1981.
- [57] R. Scheer. *Korrelation von Struktur und elektronischen Eigenschaften mehrphasiger Cu-In-S Schichten für die Photovoltaik*. PhD thesis, Technische Universität Berlin, 1993.
- [58] L. L. Kazmerski and G. A. Sanborn.  $\text{CuInS}_2$  thin-film homojunction solar cells. *J. Appl. Phys.*, 48:3178–3180, 1977.
- [59] R. Scheer, T. Walter, H. W. Schock, M. L. Fearheiley, and H. J. Lewerenz. *Appl. Phys. Lett.*, 63:3294, 1993.
- [60] H. L. Hwang, B. H. Tseng, C. Y. Sun, and J. J. Loferski. *Solar Energy Materials and Solar Cells*, 4:67, 1980.
- [61] M. Krunks, V. Mikli, O. Bijakina, and E. Millikov. Growth and recrystallization of  $\text{CuInS}_2$  films in spray pyrolytic process. *Appl. Sur. Sci.*, 142:356–361, 1999.
- [62] Z. Pei, J. S. Yu, B. H. Tseng, and H. L. Hwang. Growth and characterization of  $\text{CuIn}_x\text{Ga}_{1-x}\text{S}_2$  and  $\text{CuInS}_y\text{Se}_{2-y}$  thin films by reactive sputtering. In *Proc. of ICTMC-11, Salford*, pages 321–324, 1997.
- [63] T. Walter, D. Braunger, H. Dittrich, Ch. Köble, R. Herberholz, and W. Schock. Sequential processes for the deposition of polycrystalline  $\text{Cu}(\text{In,Ga})(\text{S,Se})_2$  thin films: Growth mechanism and devices. *Solar Energy Materials and Solar Cells*, 41/42:355–372, 1996.
- [64] K. Siemer, J. Klaer, I. Luck, J. Álvarez García, A. Perez Rodríguez, A. Romano-Rodríguez, and D. Bräunig. Growth monitoring of  $\text{CuInS}_2$  absorber layers prepared by a rapid thermal process (RTP). In *Proceedings of 16th EPVSEC, Glasgow*, 2000.
- [65] R. Klenk, U. Blieske, V. Dieterle, K. Ellmer, S. Fiechter, I. Hengel, A. Jäger-Waldau, T. Kampschulte, Ch. Kaufmann, J. Klaer, M. Ch. Lux-Steiner, D. Hariskos, M. Ruckh, and H. W. Schock. Properties of  $\text{CuInS}_2$  thin films grown by a two-step process without  $\text{H}_2\text{S}$ . *Solar Energy Materials and Solar Cells*, 49:349–356, 1997.
- [66] K. Siemer. *Schichtwachstum und elektronische Defekteigenschaften von  $\text{CuInS}_2$ -Absorberschichten aus dem sequentiellen Prozess*. PhD thesis, Freie Universität Berlin, 2000.
- [67] K. Pross. Charakterisierung von  $\text{Cu}(\text{In,Ga})\text{Se}_2$ -Schichten mit oberflächenanalytischen Methoden. Master's thesis, Fakultät für Physik der Universität Konstanz, 1997.
- [68] N. Q. Lam. Ion Bombardment Effects on the Near-surface Composition During Sputter Profiling. *Surface and Interface Analysis*, 12:65–77, 1988.
- [69] M. Powalla, A. Eicke, K. Pross, and B. Dimmler. SNMS Depth Profiling of  $\text{Cu}(\text{In,Ga})\text{Se}_2$  Absorber Layers For Solar Cells. In *Proceedings of 2nd WPVSEC, Vienna*, pages 1129–1132, 1998.
- [70] F. Frost, A. Schindler, and F. Bigl. Ion beam smoothing of indium-containing III-V compound semiconductors. *Appl. Phys. A*, 66:663–668, 1998.
- [71] F. Frost, G. Lippold, K. Otte, D. Hirsch, A. Schindler, and F. Bigl. Smoothing of polycrystalline  $\text{Cu}(\text{In,Ga})(\text{Se,S})_2$  thin films by low-energy ion-beam etching. *J. Vac. Sci. Technol. A*, 17:793–798, 1999.
- [72] A. Eicke. private communications.
- [73] G. Dagan, T. F. Cizek, and D. Cahen. Ion Migration in Chalcopyrite Semiconductors. *J. Phys. Chem.*, 96:11009–11017, 1992.

- 
- [74] R. Loudon. *Proc. Royal Soc.*, A275:218, 1963.
- [75] V.F. Agekyan, N.V. Orekhova, D. Rajab, and A. Yu. Serov. Luminescence and Raman scattering of light in some I-III-VI<sub>2</sub> crystals and their solid solutions. *Sov. Phys. Solid State*, 34:1215–1217, 1992.
- [76] I. P. Kaminow, E. Buehler, and J. H. Wernick. Vibrational Modes in ZnSiP<sub>2</sub>. *Phys. Rev. B*, 2:960–966, 1970.
- [77] W. H. Koschel and M. Bettini. Zone-Centered Phonons in A<sup>I</sup>B<sup>III</sup>S<sub>2</sub> Chalcopyrites. *Phys. Stat. Sol. (b)*, 72:729–737, 1975.
- [78] H. Tanino, T. Maeda, H. Fujikake, H. Nakanishi, S. Endo, and T. Irie. Raman spectra of CuInSe<sub>2</sub>. *Phys. Rev. B*, 45:13 323–13 330, 1992.
- [79] F.W. Ohrendorf and H. Haeuseler. Lattice Dynamics of Chalcopyrites Type Compounds. Part I. Vibrational frequencies. *Cryst. Res. Technol.*, 34(3):339–349, 1999.
- [80] F.W. Ohrendorf and H. Haeuseler. Lattice Dynamics of Chalcopyrites Type Compounds. Part II. Calculations in a Short Range Force Field Model. *Cryst. Res. Technol.*, 34(3):351–362, 1999.
- [81] F.W. Ohrendorf and H. Haeuseler. Lattice Dynamics of Chalcopyrites Type Compounds. Part III. Rigid Ion Model Calculations. *Cryst. Res. Technol.*, 34(3):363–378, 1999.
- [82] H. Matsushita, S. Endo, and T. Irie. Raman-Scattering Properties of I-III-IV<sub>2</sub> Group Chalcopyrites Semiconductors. *Jap. J. Appl. Phys.*, 31(1):18–22, 1992.
- [83] J. Härtwig, G. Höelzer, J. Wolf, and E. Förster. Remeasurement of the Profile of the Characteristic Cu K $\alpha$  Emission Line with High Precision and Accuracy. *J. Appl. Cryst.*, 26:539–548, 1993.
- [84] P. Scherrer. *Nachr. Göttinger Gesell.*, 98, 1918.
- [85] R. W. Cheary and A. Coelho. A Fundamental Parameters Approach to X-ray Line-Profile Fitting. *J. Appl. Cryst.*, 25:109–121, 1992.
- [86] H.P. Klug and L.E. Alexander. *X-Ray Diffraction Procedures*. John Wiley & Sons, second edition.
- [87] R. W. Cheary and A. Coelho. Axial Divergence in a Conventional X-ray Powder Diffractometer. I. Theoretical Foundations, II. Realization and Evaluation in a Fundamental-Parameter Profile Fitting Procedure. *J. Appl. Cryst.*, 31:851–861, 862–868, 1998.
- [88] A. Kern. Präzisionpulverdiffraktometrie: Ein Vergleich verschiedener Methoden. Master's thesis, Universität Heidelberg, 1992.
- [89] W. Parrish and A.J.C. Wilson, editors. *International Tables for X-Ray Crystallography*, volume 2, chapter Precision measurements of lattice parameters of polycrystalline specimens, pages 216–234. Kynoch Press, Birmingham, 1959.
- [90] Stephen Wolfram. *The MATHEMATICA book*. Oxford University Press, 4 edition, 1998.
- [91] A.J.C. Wilson and E. Prince, editors. *International Tables for Crystallography*, volume C. Kluwer Academic Publishers, Dordrecht/Boston/London, second edition, 1999.
- [92] D.T. Cromer and D. Liberman. Relativistic Calculation of Anomalous Scattering Factors for X Rays. *J. Chem. Phys.*, 53:1891–1898, 1970.
- [93] J.I. Polygalov and A.S. Poplavnoi. Anion shift influence on band structure of crystals with chalcopyrite lattice. *Journal de Physique, Colloque C3, supplément au no 9*, 36:C3–129, 1975.
- [94] D. Wolf and G. Müller. Kinetics of cis-formation studied in situ by thin film calorimetry. *Thin Solid Films*, 361–362:155–160, 2000.

- [95] M. Marudachalam, R.W. Birkmire, H.Hichri, J.Schultz, A. Swartzlander, and M.M. Al-Jassim. Phases, morphology, and diffusion in  $\text{CuIn}_x\text{Ga}_{1-x}\text{Se}_2$  thin films. *J. Appl. Phys.*, 82(6):2896–2905, 1997.
- [96] S. Zweigart. *Herstellung von Cu(In,Ga)Se<sub>2</sub>-Dünnschichten durch sequentielle Prozesse - Untersuchung zur Reaktionskinetik*. PhD thesis, Universität Stuttgart, 2000.
- [97] P. Berwian, D. Wolf, G. Müller, W. Stetter, and F. Karg. Investigation of phase formation in the Cu-In-Ga-Se system by thin film calorimetry and x-ray diffraction. In *Proceedings of 16th EPVSEC, Glasgow*, 2000.
- [98] Riedel. *Anorganische Chemie*, chapter 2, page 184 ff. de Gruyter, 1990. in german.
- [99] Landolt and Börnstein, editors. *Phase Equilibria, Crystallographic and Thermodynamic Data of Binary Alloys*, volume IV, 5, D. Springer Verlag.
- [100] W. Keppner, T. Klas, W. Körner, R. Wesche, and G. Schatz. Compound Formation at Cu-In Thin-film Interfaces Detected by Perturbed  $\gamma - \gamma$  Angular Correlations. *Phys. Rev. Lett.*, 54:2371–2374, 1985.
- [101] R. Roy and S.K. Sen. The formation of intermetallics in Cu/In thin films. *J. Mater. Res.*, 7:1377–1386, 1992.
- [102] C. Dzionk, H. Metzner, H. J. Lewerenz, and H. E. Mahnke. Perturbed angular correlations study of thin Cu-In films. *J. Appl. Phys.*, 78(4):2392–2397, 1995.
- [103] M. Gossila, H. Metzner, and H.-E. Mahnke. Coevaporated Cu-In films as precursors for solar cells. *J. Appl. Phys.*, 86:3624–3632, 1999.
- [104] O.I. Tikhomirova, M.V. Pikunov, I.D. Marchukova, I.N. Tochenova, and I.P. Izotova. An investigation of structural transformation during the solidification of copper-gallium alloys. *Sov. Mater. Science*, 5:355–358, 1969.
- [105] O.I. Tikhomirova, L.P. Ruzinov, M.V. Pikunov, and I.D. Machukova. *Fiz. Met. Metalloved*, 29:796, 1970. in Russian.
- [106] A. Hartmann. Formation, Characterization and Analysis of Sputtered Cu/In and CuGa/In Bilayers for use in Photovoltaic Devices. Master’s thesis, Universität Stuttgart in conjunction with University of Delaware, 1993.
- [107] E. G. Villora. Charakterisierung und Optimierung der Mikrostrukture von  $\text{CuInS}_2$ - Dünnschichten. Master’s thesis, Technische Universität Berlin, 1998.
- [108] E. G. Villora, S. Fiechter, R. Klenk, and M. Ch. Lux-Steiner. Phase Formation and Growth Mechanism of Ternary and Quaternary  $\text{Cu(In,Ga)S}_2$  chalcopyrite layers. In *Proc. of 12<sup>th</sup> Int. Conf. Tern. Multi. Comp.*, 2000.
- [109] M. Engelmann, B.E. McCandless, and R.W. Birkmire. Formation and Analysis of Graded  $\text{CuIn}(\text{Se}_{1-y}\text{S}_y)_2$  Films. In *Proc. of EMRS, Strasbourg*, 2000.
- [110] L. Calvo-Barrio, A. Pérez-Rodríguez, J. Alvarez-García, A. Romano-Rodríguez, J.R. Morante, K. Siemer, I. Luck, R. Klenk, and R. Scheer. Combined In-Depth Scanning Auger Microscopy and Raman Scattering Characterisation of  $\text{CuInS}_2$  Polycrystalline Films. In *presented at the 20<sup>th</sup> Int. Seminar on Surf. Phys., Kudowa Zdroj, Poland*, 2000.
- [111] J.J.M. Binsma, L.J. Giling, and J. Bloem. Phase Relations in the system  $\text{Cu}_2\text{S-In}_2\text{S}_3$ . *J. Cryst. Growth*, 50:429–436, 1980.
- [112] A. Zunger. *Appl. Phys. Lett.*, 50:164, 1987.

- 
- [113] G. Eriksson and K. Hack. Chemsage - a computer program for the calculation of complex chemical equilibria. *Metallurgical Transactions B*, 21:1013, 1990.
- [114] C. Dzionk, H. Metzner, S. hessler, and H. E. Mahnke. Phase formation during the reactive annealing of Cu-In films in H<sub>2</sub>S atmosphere. *Thin Solid Films*, 299:38–44, 1997.
- [115] R. Klenk, T. Walter, D. Schmid, and H.W. Schock. Growth Mechanism and Diffusion in Multinary and Multilayer Chalcopyrite Thin Films. *Jap. J. Appl. Phys.*, 32-3:57, 1993.
- [116] F. Karg, V. Porbst, H. Harms, J. Rimmasch, W. Riedl, J. Kotschy, J. Holz, R. Treichler, O. Eibl, A. Mitwalsky, and A. Kiendl. Novel Rapid-Thermal-Processing for CIS Thin-Film Solar Cells. In *Proc. of 23th IEEE PVSEC*, 1993.
- [117] S. Yamanaka, B. E. McCandless, and R. W. Birkmire. Reaction chemistry of CuInSe<sub>2</sub> formation by selenization using elemental Se. In *Proc. of 23<sup>rd</sup> IEEE PVSEC*, pages 607–612, 1993.
- [118] D. Cahen and R. Noufi. Free Energies and Enthalpies of Possible Gas Phase and Surface Reactions for Preparation of CuInSe<sub>2</sub>. *J. Phys. Chem. Solids*, 52:947–961, 1991.
- [119] C. Köble. Herstellung und Charakterisierung von CuInS<sub>2</sub>-Schichten für die photovoltaische Anwendung. Master's thesis, Universität Stuttgart, 1994.
- [120] M. Kleinfeld and H.-D. Wiemhöfer. Chemical Diffusion Coefficients and Stability of CuInS<sub>2</sub> and CuInSe<sub>2</sub> from Polarization Measurements with Point Electrodes. *Solid-State Ionics*, 28–30:1111–1115, 1988.
- [121] S. Wißman and K.D. Becker. Tracer diffusion of indium in CuInS<sub>2</sub>. *Solid State Ionics*, 101–103:539–545, 1997.
- [122] H. J. Bardeleben, A. Goltzené, and C. Schwab. ESR assessment of sulphur diffusion in CuGaS<sub>2</sub>. *Inst. Phys. Conf. Ser.*, 35:43–50, 1977.
- [123] H.J. von Bardeleben. Selenium self-diffusion study in the 1-3-6<sub>2</sub> semiconductor: CuInSe<sub>2</sub>. *J. Appl. Phys.*, 56:321–326, 1984.
- [124] A. Zunger, S. B. Zhang, and S-H. Wei. Revisiting the defect physics in CuInSe<sub>2</sub> and CuGaSe<sub>2</sub>. In *Proc. 26<sup>th</sup> IEEE PVSC*, 1997.
- [125] C. Wagner. The evaluation of data obtained with diffusion couples of binary single-phase and multiphase systems. *Acta Metall.*, 17:99–107, 1969.
- [126] C. L. Jensen, d. E. Tarrant, J. H. Ermer, and G. A. Pollock. The Role of Gallium in CuInSe<sub>2</sub> Solar Cells Fabricated by a Two-Stage Process. In *Proc. 23rd IEEE PVSEC*, pages 577–579, 1993.
- [127] D. S. Su and S. H. Wei. Transmission electron microscopy investigation and first-principles calculation of the phase stability in epitaxial CuInS<sub>2</sub> and CuGaSe<sub>2</sub> films. *Appl. Phys. Lett.*, 74:2483–2485, 1999.
- [128] R. Hunger. *Molekularstrahlepitaxie von Kuperindiumsulfid auf Silizium*. PhD thesis, Fachbereich Physik, Technische Universität Berlin, 1999.
- [129] G. Wagner, D. Oppermann, K. Bente, J. Lenzner, and M. Lorenz. CuAu-I type ordering and orientation domains in tetragonal Zn<sub>2–2x</sub>Cu<sub>x</sub>In<sub>x</sub>S<sub>2</sub> films (0.78 ≤ x ≤ 1) crystallized on j(001) gallium phosphide by pulsed laser deposition. *Thin Solid Films*, 376:82–88, 2000.
- [130] B.J. Stanbery, S. Kincal, S. Kim, T.J. Anderson, and O.D. Crisalle. Role of sodium in the control of defect structures in CIS. In *Proc. of 28th IEEE PVSC, Anchorage, AK, USA*, 2000.
- [131] J. Álvarez García, J. Marcos-Ruzafa, A. Pérez-Rodríguez, A. Romano-Rodríguez, J. R. Morante, and R. Scheer. Microraman Scattering from Polycrystalline CuInS<sub>2</sub> Films: Structural Analysis. *Thin Solid Films*, 1999. in press.

- [132] J. Álvarez García, A. Pérez-Rodríguez, A. Romano-Rodríguez, T. Jawhari, J. R. Morante, and R. Scheer. Raman Scattering structural evaluation of CuInS<sub>2</sub> thin films. In *Proc. of EMRS, Strasbourg*, 2000.
- [133] J. S. Park, Z. Dong, S. Kim, and J. H. Perepezko. CuInSe<sub>2</sub> phase formation during Cu<sub>2</sub>Se/In<sub>2</sub>Se<sub>3</sub> interdiffusion reaction. *J. Appl. Phys.*, 87(08):3683–3690, 2000.
- [134] M. Marudachalam, H. Hichri, R.W. Birkmire, and J.M. Schultz. Diffusion of In and Ga in selenized Cu-In and Cu-Ga precursors. In *Proceedings of 25<sup>th</sup> PVSC, Washington, D.C.*, pages 805–807, 1996.
- [135] J. Álvarez García, A. Pérez-Rodríguez, A. Romano-Rodríguez, J. R. Morante, L. Calvo-Barrio, R. Scheer, and R. Klenk. Microstructure and secondary phases in coevaporated CuInS<sub>2</sub> films: Dependence on growth temperature and chemical composition. *J. Vac. Sci. Technol.*, A19:232, 2001.
- [136] M. Marudachalam. *Processing, structure and diffusion in CuIn<sub>x</sub>Ga<sub>1-x</sub>Se<sub>2</sub> thin films for solar cells*. PhD thesis, Faculty of Materials Science, University of Delaware, U.S.A., 1996.
- [137] B.I. Boltaks. *Diffusion in Semiconductors*, chapter IV. Infosearch Limited London, 1963.
- [138] G. H. Gilmer and H. H. Farrell. Grain-boundary diffusion in thin films. II. Multiple grain boundaries and surface diffusion. *J. Appl. Phys.*, 47(10):4373–4380, 1976.
- [139] I. Kaur, Y. Mishin, and W. Gust. *Fundamentals of Grain and Interphase Boundary Diffusion*. John Wiley & Sons Ltd, 1995.
- [140] D. Shaw. *Atomic diffusion in semiconductors*, chapter General features of diffusion in semiconductors. Plenum Press, London and New York, 1973.
- [141] D. J. Schroeder, G. D. Berry, and A. A. Rockett. Gallium diffusion and diffusivity in CuInSe<sub>2</sub> epitaxial layers. *Appl. Phys. Lett.*, 69(26):4068–4070, 1996.
- [142] H. J. Lewerenz, H. Goslowsky, K.-D. Husemann, and S. Fiechter. *Nature*, 321:687, 1986.
- [143] K. W. Mitchell, G. A. Pollock, and A. V. Mason. In *Proc. of 20<sup>th</sup> IEEE PVSEC, Las Vegas*, 1988.
- [144] R. Scheer, M. Alt, I. Luck, and H.J. Lewerenz. Electrical Properties of Coevaporated CuInS<sub>2</sub> Thin Films. *Solar Energy Materials and Solar Cells*, 49:423, 1997.
- [145] D. Braunger, Th. Dürr, D. Hariskos, Ch. Köble, Th. Walter, N. Wieser, and H. W. Schock. Improved open circuit voltage in CuInS<sub>2</sub>-based solar cells. In *Proceedings of 25<sup>th</sup> PVSC, Washington, D.C.*, pages 1001–1004, 1996.
- [146] D. Braunger, D. Hariskos, T. Walter, and H. W. Schock. An 11.4% efficient polycrystalline thin film solar cell based on CuInS<sub>2</sub> with a Cd-free buffer layer. *Solar Energy Materials and Solar Cells*, 40:97–102, 1996.
- [147] A. M. Chaparo, R. Bayón, M. T. Gutiérrez, J. Herrero, J. Klaer, K. Siemer, and D. Bräunig. Comparative Study of high efficiency thin film solar cells based on CuInS<sub>2</sub> absorber and alternative buffer layers. In *Proceedings of 16<sup>th</sup> EPVSEC, Glasgow*, 2000.
- [148] R. Bayón, J. Herrero, and J. Klaer. Optical properties of CBD-InZn<sub>x</sub>(OH,S) buffer thin films for photovoltaic applications. In *Proceedings of 16<sup>th</sup> EPVSEC, Glasgow*, 2000.
- [149] I. Hengel, R. Klenk, E. García Villora, and M. Ch. Lux-Steiner. Isovalent and non-isovalent substitutions in CuInS<sub>2</sub>. In *In Proceedings of 2<sup>nd</sup> WPVSEC*, 1998.
- [150] N. G. Dhere and S. R. Ghongadi. CIGS<sub>2</sub> Thin Film Solar Cells On Stainless Steel Foil. In *Mat. Res. Soc. Symp. Proc.*, volume 668, page H3.4.1. Materials Research Society, 2001.
- [151] S. B. Zhang, S.-H. Wei, and A. Zunger. Stabilization of Ternary Compounds via Ordered Arrays of Defect Pairs. *Phys. Rev. Lett.*, 78:4059–4062, 1997.



- 
- [152] S. B. Zhang, S.H. Wei, and A. Zunger. A phenomenological model for systematization and prediction of doing limits in II-VI and I-III-VI<sub>2</sub> compounds. *J. Appl. Phys.*, 83:3192–3196, 1997.
- [153] A. Klein and W. Jaegermann. Fermi-level-dependent defect formation in Cu-chalcopyrite semiconductors. *Appl. Phys. Lett.*, 74:2283–2285, 1999.
- [154] I. Luck, M. Weber, H.-J. Lewerenz, and R. Scheer. Improved open circuit voltage of 841 mV of thin film solar cells based on a Zn<sub>2–2x</sub>Cu<sub>x</sub>In<sub>x</sub>S<sub>2</sub> absorber layer. In *Proc. of 2<sup>nd</sup> WCPEC, Vienna*, pages 549–552, 1998.
- [155] A. Werner, I. Luck, J. Bruns, J. Klaer K. Siemer, and D. Bräunig. Investigation of the influence of silver on the growth mechanism of CuInS<sub>2</sub>. *Thin Solid Films*, 361–362:88–92, 2000.
- [156] R. Scheer, M. Alt, I. Luck, R. Schiek, and H.-J. Lewerenz. Electrical properties of coevaporated CuInS<sub>2</sub> films by in-situ conductivity measurements. In *Proc. Mater. Res. Soc.*, pages 309–314, 1996.
- [157] I. Luck, J. Kneisel, K. Siemer, J. Bruns, R. Scheer, R. Klenk, N. Janke, and D. Bräunig. Influence of Na on the properties of Cu-rich prepared CuInS<sub>2</sub> thin films and the performance of corresponding CuInS<sub>2</sub>/CdS/ZnO solar cells. *Solar Energy Materials and Solar Cells*, 67:151–158, 2001.
- [158] J. Klaer, J. Bruns, R. Henninger, K. Siemer, R. Klenk, K. Ellmer, and D. Bräunig. Efficient CuInS<sub>2</sub> thin-film solar cells prepared by a sequential process. *Semicond. Sci. Technol.*, 13:1456–1458, 1998.
- [159] R. Hulstrom, R. Bird, and C. Riordan. *Solar Cells*, 15:395, 1985.
- [160] J. Kneisel, K. Siemer, I. Luck, and D. Bräunig. Admittance spectroscopy of efficient CuInS<sub>2</sub> thin film solar cells. *J. Appl. Phys.*, 88:5474, 2000.
- [161] J. Reiss, J. Malmström, A. Werner, I. Hengel, R. Klenk, and M.Ch. Lux-Steiner. Current Transport in CuInS<sub>2</sub> Solar Cells Depending on Absorber Preparation. In *Mat. Res. Soc. Symp. Proc.*, volume 668, page H.9.4.1, 2001.
- [162] A. Klein, T. Löher, Y. Tomm, C. Pettenkofer, and W. Jaegermann. Band lineup between CdS and ultra high vacuum-cleaved CuInS<sub>2</sub> single crystals. *Appl. Phys. Lett.*, 70:1299–1301, 1997.
- [163] Y. Hashimoto, K. Takeuchi, and K. Ito. Band alignment at CdS/CuInS<sub>2</sub> heterojunction. *Appl. Phys. Lett.*, 67:980–983, 1995.
- [164] R. Scheer, I. Luck, and H.J. Lewerenz. In *Proceedings of the 12th EPVSEC, Amsterdam*, page 1751, 1994.
- [165] R. Scheer. Interface and surface properties of ternary semiconductors. In *Proc. of 12<sup>th</sup> ICTMC, Taiwan*, 2000.
- [166] D.S. Albin. *Fabrication and Structural, Optical, and Electrical Characterization of Multi-Source Evaporated Copper Gallium Selenide Polycrystalline Thin Films*. PhD thesis, Department of Material Science and Engineering, The University of Arizona, 1989.
- [167] L. G. Harrison. *Trans. Faraday Soc.*, 57:1191, 1961.
- [168] S. Haussühl. *Kristallstrukturbestimmung*. Weinheim: Physik-Verlag; Weihheim: Verlag Chemie, 1979.
- [169] B.E. Warren. *X-ray diffraction*. Addison-Wesley Publishing company, Reading Massachusetts, 1969.
- [170] M. Kokta, J. R. Carruthers, M. Gfasso, H. M. Kasper, and B. Tell. Ternary phase relations in the vicinity of chalcopyrite copper gallium sulfide. *J. Elec. Mat.*, 5:69–89, 1976.



# Publications

Parts of this work have already been published:

## Journal Publications

- I. Hengel, A. Neisser, R. Klenk, M. Ch. Lux-Steiner.  
Current transport in CuInS<sub>2</sub>:Ga/CdS/ZnO-solar cells.  
*Thin Solid Films*. 361–362:458–462, 2000
- A. Neisser, I. Hengel, R. Klenk, Th.W. Matthes, J. Alvarez-García and A. Perez-Rodríguez, A. Romano-Rodríguez, M.-Ch. Lux-Steiner.  
Effect of Ga incorporation in sequentially prepared CuInS<sub>2</sub> thin film absorbers.  
*Solar Energy Materials and Solar Cells*. 67:97–104, 2001.
- J. Alvarez-García, J.R. Morante, A. Perez-Rodríguez, A. Romano-Rodríguez, L. Calvo-Barrio, R.Scheer, R. Klenk, A. Neisser.  
Raman scattering from CuInS<sub>2</sub> and Cu(InGa)S<sub>2</sub> thin films.  
*Asian J. Phys.* in press, 2001.

## Conference Proceedings

- A. Neisser, J. Alvarez-García, L. Calvo-Barrio, R. Klenk, Th.W. Matthes, I. Luck, M.Ch. Lux-Steiner, A. Pérez-Rodríguez, J.R. Morante.  
Cu(In,Ga)S<sub>2</sub> Phase Formation from Metallic Cu-In-Ga Precursor Stacks in Rapid Thermal Processes.  
*Mat. Res. Soc. Symp. Proc.* 668:H.1.3.1, 2001.
- Th. Riedle, Th.W. Matthes, A. Neisser, R. Klenk, C. Hinrichs, N. Esser, W. Richter, M. Ch. Lux-Steiner.  
Preparation of CuInS<sub>2</sub> absorber layers by rapid thermal sulfurization using H<sub>2</sub>S and DTBS.  
*Proceedings of 16th EPVSEC, Glasgow*:713–716, 2000.

## Poster Presentations

- Th. Riedle, A. Neisser, K. Otte, R. Klenk, N. Esser, W. Richter, M. Ch. Lux-Steiner.  
Ramanspektroskopie an dünnen Cu(In,Ga)S<sub>2</sub> - Absorberschichten für Solarzellen.  
presented at DPG Frühjahrstagung, Hamburg, 2001.

