Strong increase of the electron effective mass in GaAs incorporating boron and indium

Ellipsometry Workgroup

UNIVERSITÄT LEIPZIG

T. Hofmann[#,1)], C. v. Middendorff[1)], G. Leibiger[2)], V. Gottschalch[2)], and M. Schubert[1)]

1) Institut für Experimentelle Physik II, Fakultät für Physik und Geowissenschaften, Universität Leipzig

2) Institut für Anorganische Chemie, Fakultät für Chemie und Mineralogie, Universität Leipzig

[#]E-mail: Tino.Hofmann@physik.uni-leipzig.de

HL 12.50

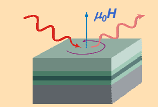
Our message

The novel low band-gap material BInGaAs shows obscure band structure properties:

- Strong increase of the Γ-point optical effective electron mass on incorporating of B and In
- Unexpected increase of the effective electron mass with decreasing free-charge-carrier concentration

Non-contact, optical determination of the free-charge-carrier parameters concentration, effective mass, and mobility in layered structures:

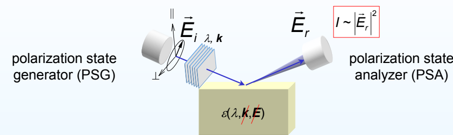
Fir MO-ellipsometry



Contacts: NO!
Heterostructures: YES!

see also Poster HL 12.90!

Experimental setup



polarization state generator (PSG)

polarization state analyzer (PSA)

Model-dielectric function

Polar lattice contribution

Electronic contribution	Infrared-active phonon modes	Alloy-induced modes	Free-carrier contribution

$$\varepsilon_j(\omega,H) = \varepsilon_{\infty,j} \cdot \prod_{i=1}^{l} \frac{\omega^2 + i\gamma_{LO,ij}\omega - \omega_{LO,ij}^2}{\omega^2 + i\gamma_{TO,ij}\omega - \omega_{TO,ij}^2} \cdot \prod_{k=1}^{m}\left(1 + \frac{i\delta\gamma_{kj}\,\omega - \delta\omega_{kj}^2}{\omega^2 + i\gamma_{AM,kj}\omega - \omega_{AM,kj}^2}\right) - \varepsilon_j^{(FC-MO)}(\omega,H)$$

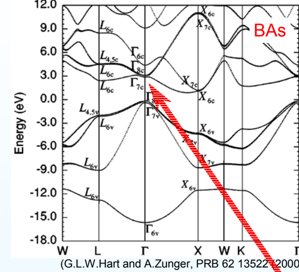
- Infrared-active phonon modes:
  $\omega_{TO/LO}$ – TO/LO phonon mode frequency
  $\gamma_{TO/LO}$ – TO/LO broadening parameter
- alloy-induced modes:
  ($\omega_{TO} - \omega_{LO} << \omega_{TO}$, ω_{LO})
  $\delta\omega_k = \omega^2_{LO,k} - \omega^2_{TO,k}$, $\gamma_{AM,k} = \gamma_{TO,k}$, and $\omega_{AM,k} = \omega_{LO,k}$
- Free-carrier contribution:
  $\omega_{p,j} \propto \zeta_j = (N/m^*_j)^{0.5}$ – plasma frequency
  $\gamma_{p,j} \propto \xi_j = (m^*_j \mu_j)^{-1}$ – scattering tensor
  N – free-carrier concentration
  m^*_j – free-carrier effective mass tensor
  μ_j – free-carrier mobililty tensor

$$\varepsilon_j^{(FC-MO)}(\omega, H=0) = \frac{\omega_{p,j}^2 \varepsilon_{\infty,j}}{\omega(\omega + i\gamma_{p,j})}$$

ε has tensor-character if H≠0!

BInGaAs – a new low band-gap material

BInGaAs is a candidate for the 1eV band-gap absorber material in tandem solar cells with a widely unknown band structure!

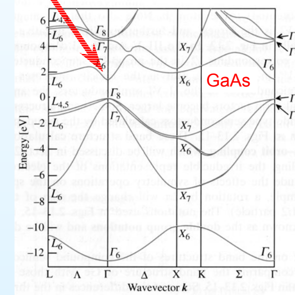


(G.L.W.Hart and A.Zunger, PRB 62 13522 (2000))

Relativistic energy-band structure of BaAs (indirect). The lowest Brillouin-zone center conduction band of BAs has *p* symmetry (Γ_{15c}, like Si) rather than *s* symmetry (Γ_{1c}, like GaAs or InAs).

first calculations indicate:

- small band-gap bowing in the BGaAs-alloy (compared to GaAsN)
- addition of B in GaAs and InGaAs *increases* the band-gap
- BGaAs behavior differs qualitatively from GaAsN



(P.Y.Yu and M. Cardona, Springer 1996)

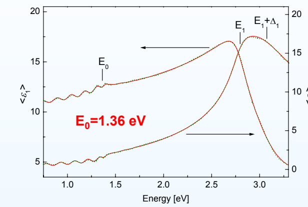
Solar cell device

Design of a low band-gap solar cell based on BInGaAs as absorber material: **see also Poster HL 44.55 on Thursday**.

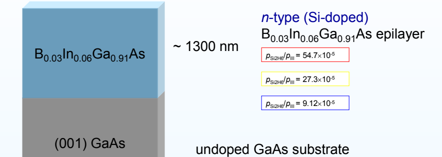
Layer	Function	Doping	N
GaAs	Cap-layer	p-doped	N=5*10^{18} cm^{-3}
GaInP	Window	p-doped	N=5*10^{16} cm^{-3}
GaAs	Emitter	p-doped	N=1.5*10^{18} cm^{-3}
BInGaAs	Base	n-doped	N=2*10^{16} cm^{-3}
GaInP		n-doped	N=1.1*10^{17} cm^{-3}
GaAs	Buffer	n-doped	N=1.5*10^{17} cm^{-3}
(001) GaAs	Substrate	n-doped	

n-type BInGaAs with different Si concentrations

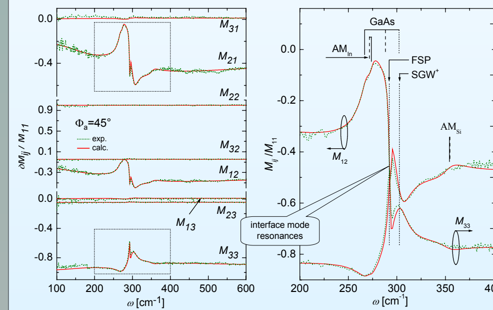
NIR-VIS ellipsometry



Measured real $<\varepsilon_1>$ and imaginary $<\varepsilon_2>$ part of the pseudodielectric function of the sample with the highest Si-concentration. The solid lines represent the model analysis using the model dielectric function of Adachi.

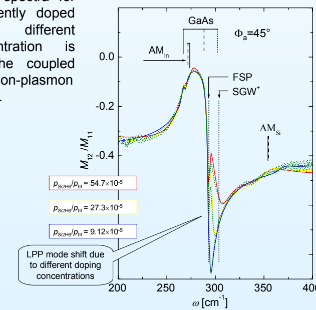


Fir generalized ellipsometry

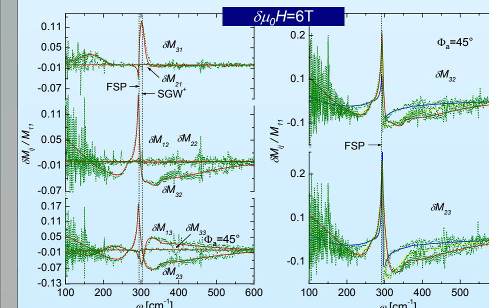


Mueller matrix elements normalized to M_{11}. Dominant structures originate from the GaAs-like Reststrahlen-band and the excitation of interface modes. The TO and LO phonon modes of the GaAs substrate can be recognized at ~268 and ~292 cm^{-1}.

Comparison of the normalized M_{12} spectra for all three, differently doped samples. The different doping concentration is evident from the coupled longitudinal-phonon-plasmon mode (LPP) shift.



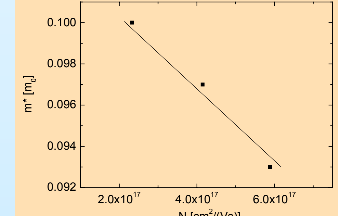
Fir-mo generalized ellipsometry



The differences of the Mueller matrix elements measured at $\mu_0 H$=-3.0T and $\mu_0 H$=3.0T represent the magnetic field induced changes of the ellipsometry data.

m [m$_0$]	*N* [10^{17} cm^{-3}]	μ [cm^2/(Vs)]
GaAs		
0.067		
B$_{0.037}$In$_{0.06}$Ga$_{0.903}$As:Si		
0.093±0.003	5.9±0.3	888±22
0.097±0.003	4.1±0.2	976±19
0.100±0.004	2.3±0.3	803±20
InAs		
0.023		

First measurement of the effective electron mass in BInGaAs!



New Data:
- first measurement of m* in B$_{0.037}$In$_{0.06}$Ga$_{0.903}$As.
- strong increase of m* compared to GaAs or InAs.
- unexpected m*(N) behavior!

T. Hofmann, G. Leibiger, N. Ashkenov, and M. Schubert Phys. Rev. Lett. submitted

Unterstützt durch die Deutsche Forschungsgemeinschaft

Gedruckt im Universitätsrechenzentrum Leipzig