

DFT calculation of the electron-density response in GaAs to an 'external electric field'

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Introduction

In the recent years, experiments were performed to probe theoretical concepts of electric screening in isolators on a microscopic scale.

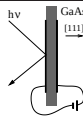
Outcome:

- The response of the charge density to the external electric field is dominated by the displacement of the Ga and As sublattices relative to each other.
- No explanation for the anisotropy in $(\Delta R/R)(E)$ (see figures below) was found.

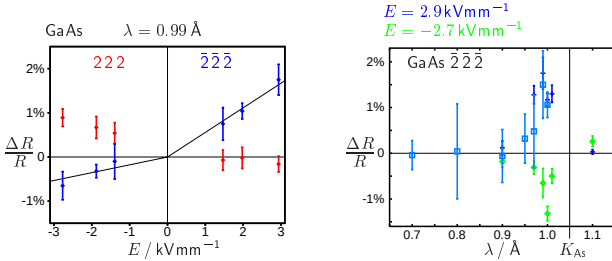
⇒ LAPW calculations with WIEN97 were performed to find an explanation.

Experiment

Determination of the relative intensity variation $\Delta R/R$ of weak reflections of GaAs caused by an homogenous externally applied electric field. The measurements were performed at HASYLAB, D3 with different wavelengths. [1]

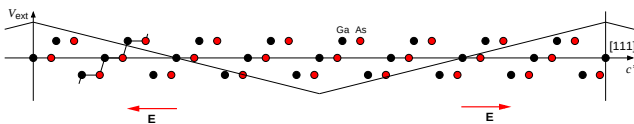


Typical results:

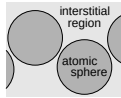


Calculations

- DFT-program: WIEN97
- the code was modified to simulate an external electrical field by addition of a periodic potential V_{ext} to the ESP.
- V_{ext} is constructed of a series of cosine functions.
- the supercell (SZ) contains 48 atoms:



- space is separated into spheres around the atoms and the remaining interstitial region.
- calculation of the structure factors F by using the quasi-atomic structure factors f_i from the spheres i located near $z = 0.25$ or $z = 0.75$, respectively.



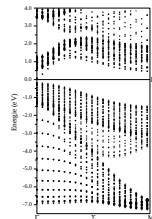
Problems, approximations

- SZ ⇒ limited resolution in k-space
- limited accuracy due to numerical reasons
⇒ field strength is 100 times larger than in the experiment
- underestimation of band gaps by LDA-DFT: isolating property has to be checked
- muffin tin potential: interstitial region is not considered in F
- calculation of $\Delta R/R$: inclusion of
— anomalous dispersion ($f'(\lambda) + i f''(\lambda)$)
— thermal effects (Debye-Waller factor T)

$$\Delta R/R \approx (|F_E|^2 - |F_0|^2) / |F_0|^2$$

$$F \approx (f_{\text{Ga}} + f'_{\text{Ga}}(\lambda) + i f''_{\text{Ga}}(\lambda)) T_{\text{Ga}} + (f_{\text{As}} + f'_{\text{As}}(\lambda) + i f''_{\text{As}}(\lambda)) T_{\text{As}} e^{ikr}$$

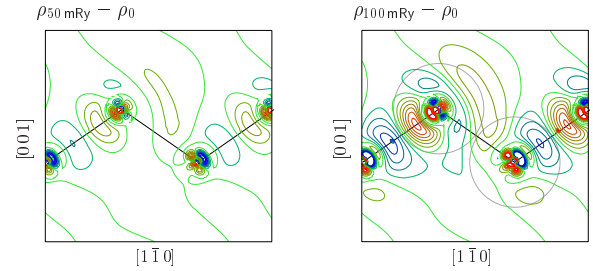
$$r = r(E), f_i = f_i(E)$$



Results

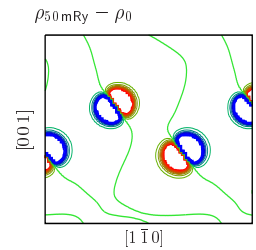
Clamped ion geometrie

- calculations for $\hat{V}_{\text{ext}} = 0, 50$ and 100 mRy ($0, 350$ and 700 kVmm $^{-1}$)
- ⇒ reproduction of Resta's results [2].
- $\Delta R/R < 10^{-3}$
- Difference charge densities, $E \parallel [\bar{1}\bar{1}\bar{1}]$

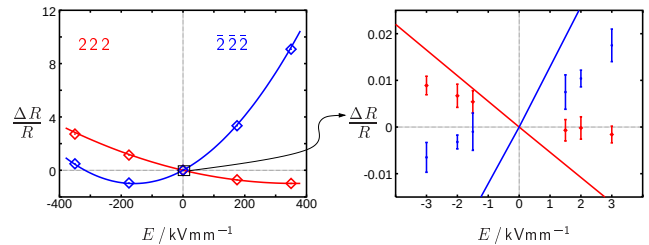


Relaxed ion positions

- criteria: no forces on the nuclei
- ⇒ $\Delta(r_{\text{As}} - r_{\text{Ga}}) = 0.01 \text{ \AA}$ ($\hat{V}_{\text{ext}} = 50$ mRy)
- $\Delta \rho_r$ fixed is not altered
- Difference charge densities, $E \parallel [\bar{1}\bar{1}\bar{1}]$



- $(\Delta R/R)(V_{\text{ext}})$



diamonds: results of DFT calculations

solid lines: predictions of calculation with superposed atoms, $r = r(E)$

⇒ The effect of the redistribution of the charge density is several orders of magnitude smaller compared with the displacement of atoms

⇒ strong anisotropy of $(\Delta R/R)(E)$ is not reproduced by DFT calculations

References

- [1] Stahn J. et al.: *Electric-field-induced electron density response of GaAs and ZnSe*, Europhys. Lett. **44**, 714-20 (1998).
- [2] Resta R. & Baldereschi A.: *Dielectric matrices and local fields in polar semiconductors*, Phys. Rev. B **23**, 6615-24 (1981).

Acknowledgements

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