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.

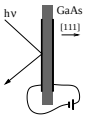
Outcome:

- 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.

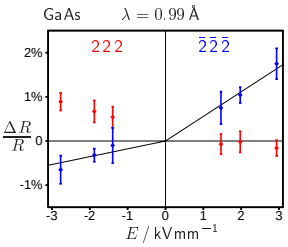
⇒ LAPW calculations with WIEN97 were performed to find an explanation.

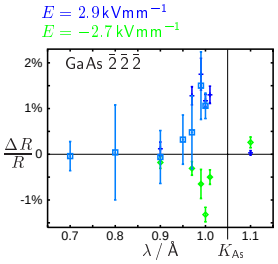
Experiment

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



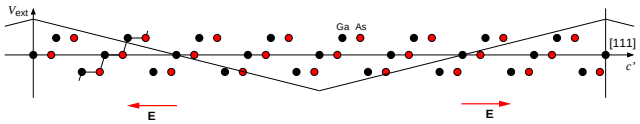
Typical results:



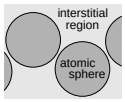


Calculations

- 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:

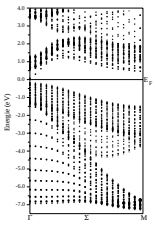


- space is separated into spheres around the atoms and the remaining interstitial region.
- calculation of the structure factors F by using the quasi-atomic structure factors f_i from the spheres i located near $z = 0.25$ or $z = 0.75$, respectively.



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 $(f'(\lambda) + \mathrm{i}\, f''(\lambda))$
  — thermal effects (Debye-Waller factor T)



$$\Delta R/R \approx \left(|F_{\mathrm{E}}|^2 - |F_0|^2\right) / |F_0|^2$$

$$F \approx \left(f_{\mathrm{Ga}} + f'_{\mathrm{Ga}}(\lambda) + \mathrm{i}\, f''_{\mathrm{Ga}}(\lambda)\right) T_{\mathrm{Ga}} + \left(f_{\mathrm{As}} + f'_{\mathrm{As}}(\lambda) + \mathrm{i}\, f''_{\mathrm{As}}(\lambda)\right) T_{\mathrm{As}}\, \mathrm{e}^{\mathrm{i}\mathbf{kr}}$$

$\mathrm{r} = \mathrm{r(E)}$, $f_i = f_i(\mathrm{E})$

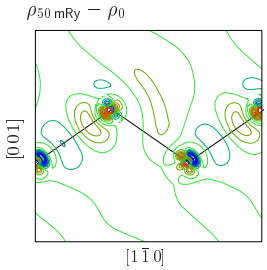
Results

Clamped ion geometrie

- calculations for $\hat{V}_{\text{ext}} = 0,\ 50$ and 100 mRy $(0,\ 350$ and $700\,\mathrm{kVmm^{-1}})$

⇒ reproduction of Resta's results [2].

- $\Delta R/R < 10^{-3}$
- Difference charge densities, E$\|[\bar{1}\,\bar{1}\,\bar{1}]$

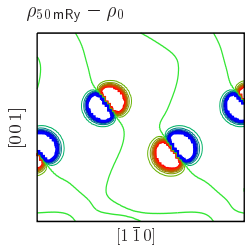


Relaxed ion positions

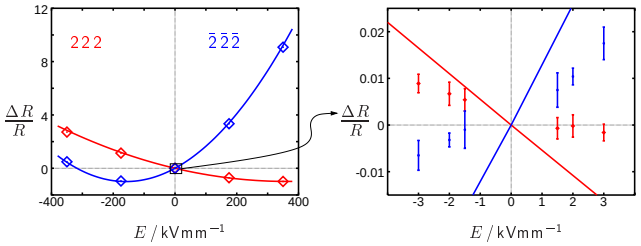
- criteria: no forces on the nuclei

⇒ $\Delta(\mathrm{r_{As}} - \mathrm{r_{Ga}}) = 0.01$ Å $(\hat{V}_{\text{ext}} = 50$ mRy)

- $\Delta\rho_{r\ \text{fixed}}$ is not altered
- Difference charge densities, E$\|[\bar{1}\,\bar{1}\,\bar{1}]$ ⟶



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



dianonds: 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),

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