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 insulators 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 with HASYLAB, D3 with different wavelengths. [1]

Typical results:

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

Calculations

- \((\Delta R / R)(V_{\text{ext}})\)
- space is separated into spheres around the atoms and the remaining interstitial region.
- calculation of the structure factors \(F^\ast\) 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

- \(S|Z\) \Rightarrow limited resolution in \(k\)-space
- limited accuracy due to numerical reasons
- \(f\)-field strength is 100 times larger than in the experiment
- underestimation of band gaps by LDA-DFT: isolating potential has to be checked
- muffin tin potential: interstitial region is not considered in \(F^\ast\)
- calculation of \(\Delta R / R\): inclusion of
  - anomalous dispersion \((f_0^\ast(\lambda) + i f_1^\ast(\lambda))\)
  - thermal effects (Debye-Waller factor \(T\))

\(\Delta R / R \approx [ (F_{\text{DW}}^2 - |F_0|^2) / |F_0|^2 ]\)

\(F^\ast = (f_{\text{ix}} + f_{\text{iy}}(\lambda) + if_{\text{iz}}(\lambda)) T_{\text{Ga}} + (f_{\text{ix}} + if_{\text{iy}}(\lambda) + i f_{\text{iz}}(\lambda)) T_{\text{As}} e^{i2\pi r}(E), f_i = f_i(\lambda)\)

\(r = r(E), f_i = f_i(\lambda)\)

Clamped ion geometric

- calculations for \(V_{\text{ext}} = 0, 50\) and \(100\) mRy \((0, 350\) and \(700\) kVmm\(^{-1}\))
- \(\Delta R / R < 10^{-3}\)
- Difference charge densities, \(E|[\vec{I} \vec{T}]\)

\(\rho = \rho_0\) mRy \(\Rightarrow \rho_0\) mRy \(\Rightarrow \rho_0\)

- \(\Delta R / R\) is not reproduced by DFT calculations

![Diagram](image)

Relaxed ion positions

- criteria: no forces on the nuclei
- \(\Delta f_{\text{ix}} - f_{\text{ix}} = 0.01\) mRy \(V_{\text{ext}} = 50\) mRy
- \(\Delta f_{\text{ix}}\) field is not altered
- Difference charge densities, \(E|[\vec{I} \vec{T}]\)

\(\rho = \rho_0\) mRy \(\Rightarrow \rho_0\) mRy \(\Rightarrow \rho_0\)

- \(\Delta R / R\) is not reproduced by DFT calculations

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 \((\Delta R / R)(V_{\text{ext}})\) is not reproduced by DFT calculations

References


Acknowledgements

This project was supported by the BMBF, (grant 05 6471PA) and the EC, (grant CHRXCT-920555).

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