Raman Study of Silicon Nanowires and CdSe Nanorods

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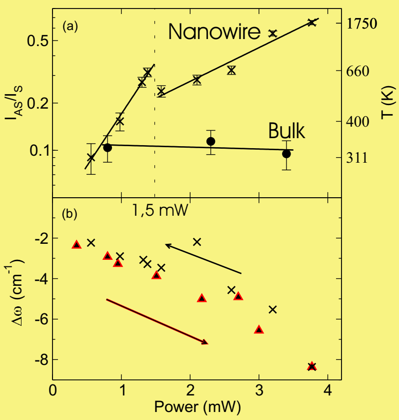
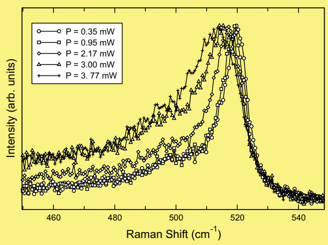
Silicon nanowires and CdSe nanorods are examined *via* Raman scattering. Investigations of the laser power, temperature and embedding gas lead to a strong dependence of thermal conductivity on surrounding gas. *Ab initio* calculations of confinement effects show good agreement with experiment. Such confinement effects may also explain the dependence of the Raman peak shape and position in CdSe Nanorods.

Raman Measurements

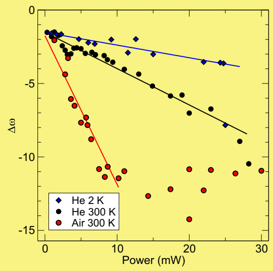


- nanowire temperature increases when irradiated with laser
- bulk temperature unchanged
- possible reconstruction of nanowire at 1,5 mW laser power

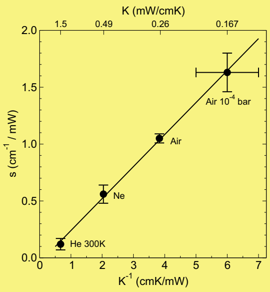
The thermal conductivity of silicon nanowires strongly depends on the surrounding gas. This is due to the high surface-to-volume ratio and the small number of points in which disordered nanowires are in contact with the substrate.



- Raman spectrum shows redshift with increasing laser power due to sample heating



- slope is proportional to the inverse of the thermal conductivity
- saturation for critical laser power



- different thermal conductivities of surrounding gases change the equilibrium temperature of the wire
- nanowires can possibly be used as gas sensors

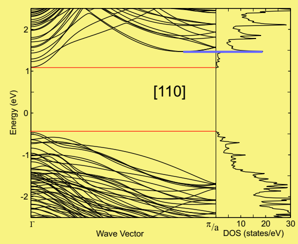
Ab initio calculations

Method:

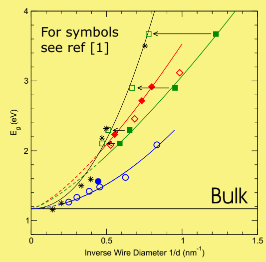
- local-density approximation
- periodic boundary conditions
- neighboring wires are separated for no interaction
- scissors operator for correct band gap of silicon

Results:

- band gap depends on growth direction of wire
- direct band gap only obtained when Γ-X-direction perpendicular to wire axis
- large DOS at Γ-point requires confinement of the bands with a transverse effective mass
- high index nanowires are indirect, only [001] nanowire is direct semiconductor



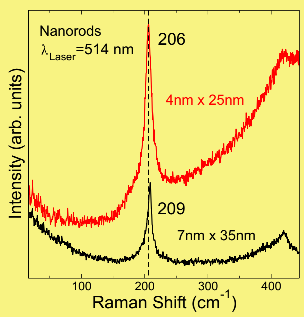
- direct band gap, but the overall character of the wire remains indirect because of small DOS in the lowest conduction band states



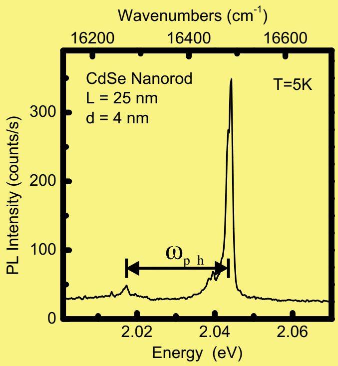
- theoretical results in good agreement with experiment when taking extension of electron wave function into account (arrows)
- enlargement of E_{gap} because of confinement

CdSe nanorods

Raman spectrum of two different sized nanorods



- spectra show different shapes and peak position, that can be due to:
  - temperature effects
  - quantization effects (zone folding)
- different background luminescence also size dependent



Luminescence spectrum of individual nanorod.

- possibly phonon sideband indicated in figure
- phonon frequency matches Raman measurements

Conclusion

- nanowires: strong dependence of Raman response on embedding gas. Application as gas sensors possible.
- electronic properties of nanowire depend on growth direction
- nanorod properties are strongly affected by size

References

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