Grain shape (and size) effects in infrared dust spectra

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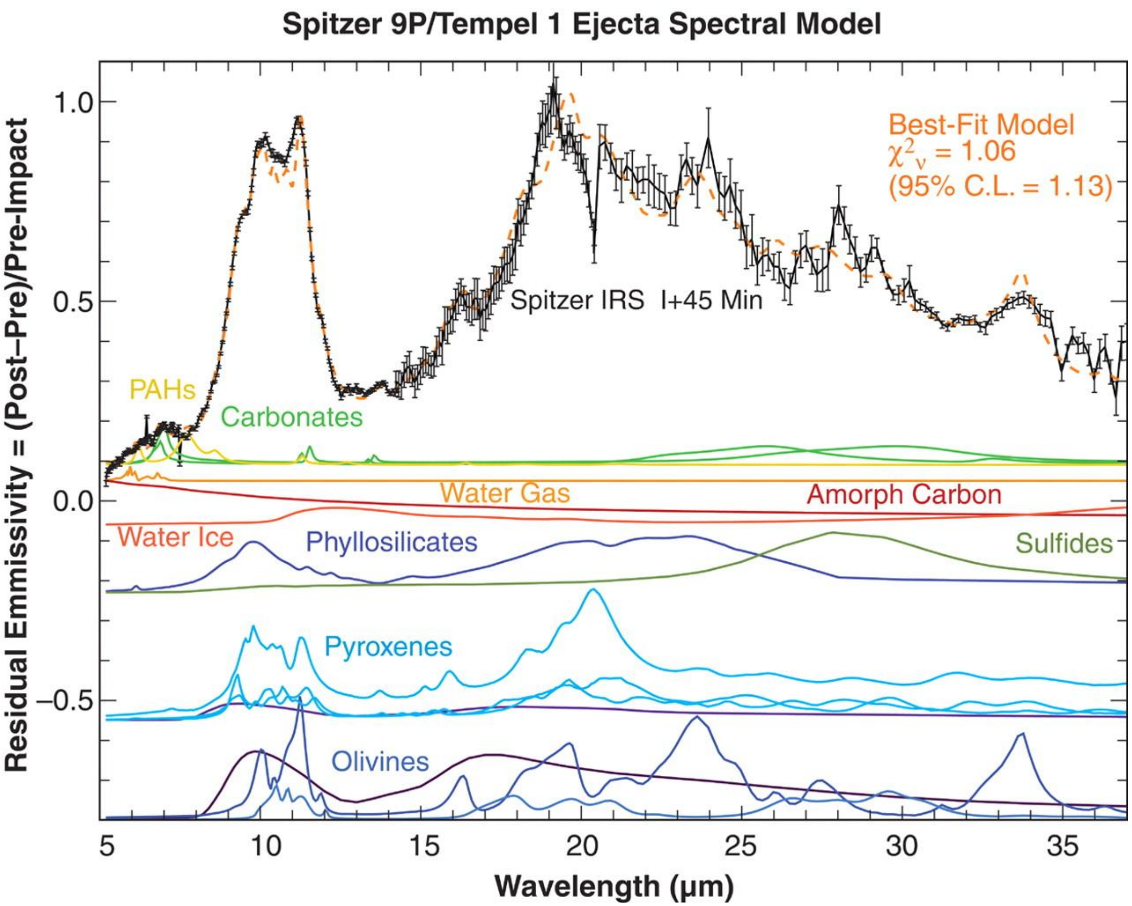
Outline

- Motivation: Comparison spectra for thermal dust emission
- Grain shape effects measured with „aerosol IR spectroscopy“
- Analysis by a „Distribution of Form Factors“ model
  (grains small compared to the wavelength)
- DDA modeling of irregular porous grains (larger grain sizes)

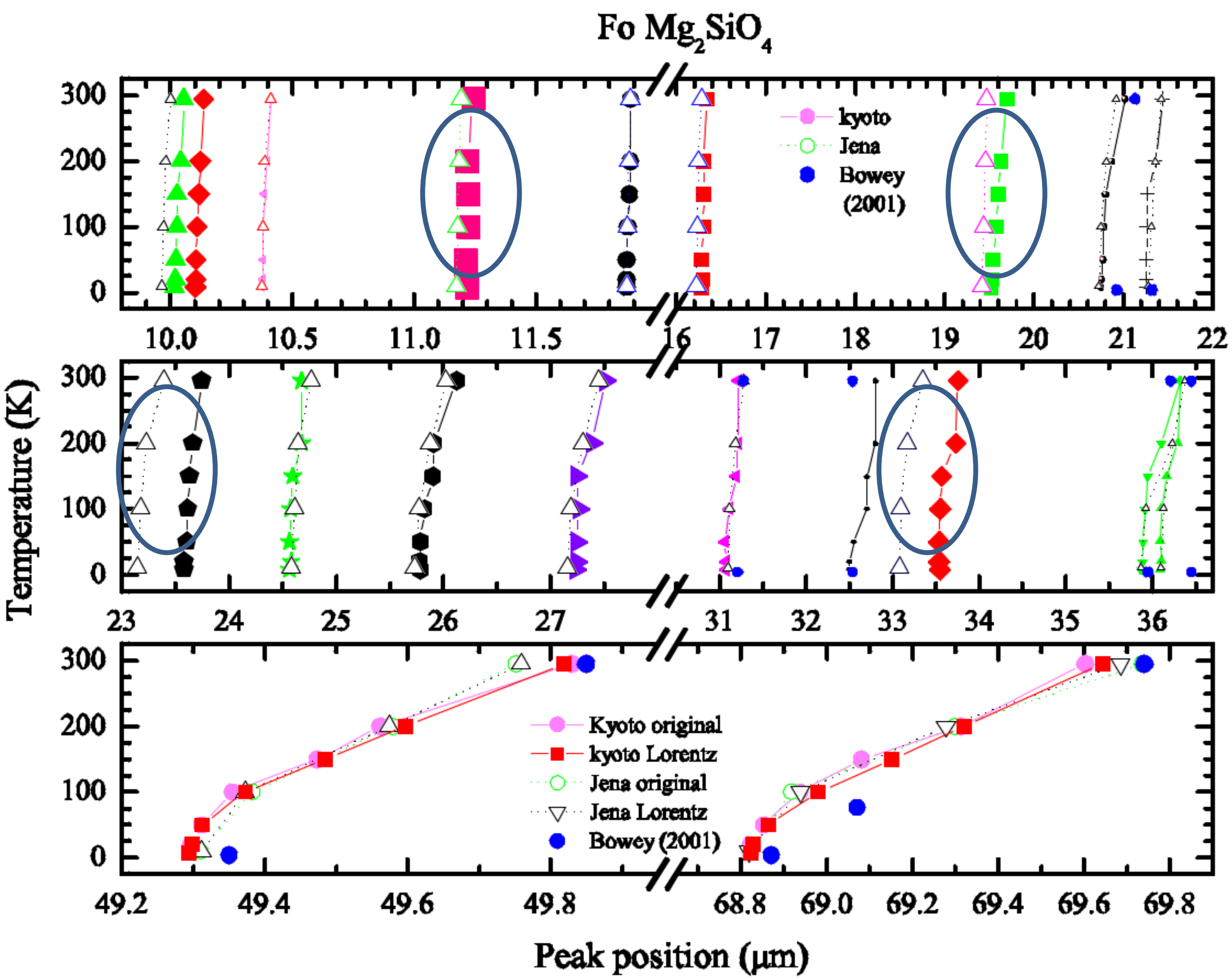
Motivation

- Mineralogy of (warm) dust can be derived from multicomponent fits of thermal emission spectra (e.g. Spitzer data)
- Comparison spectra are essential, may depend on the way they were derived



Lisse et al. (2006)

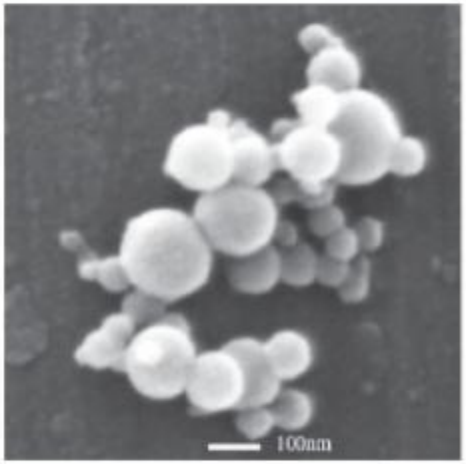
Peak positions in forsterite spectra „Kyoto sample vs. Jena sample“



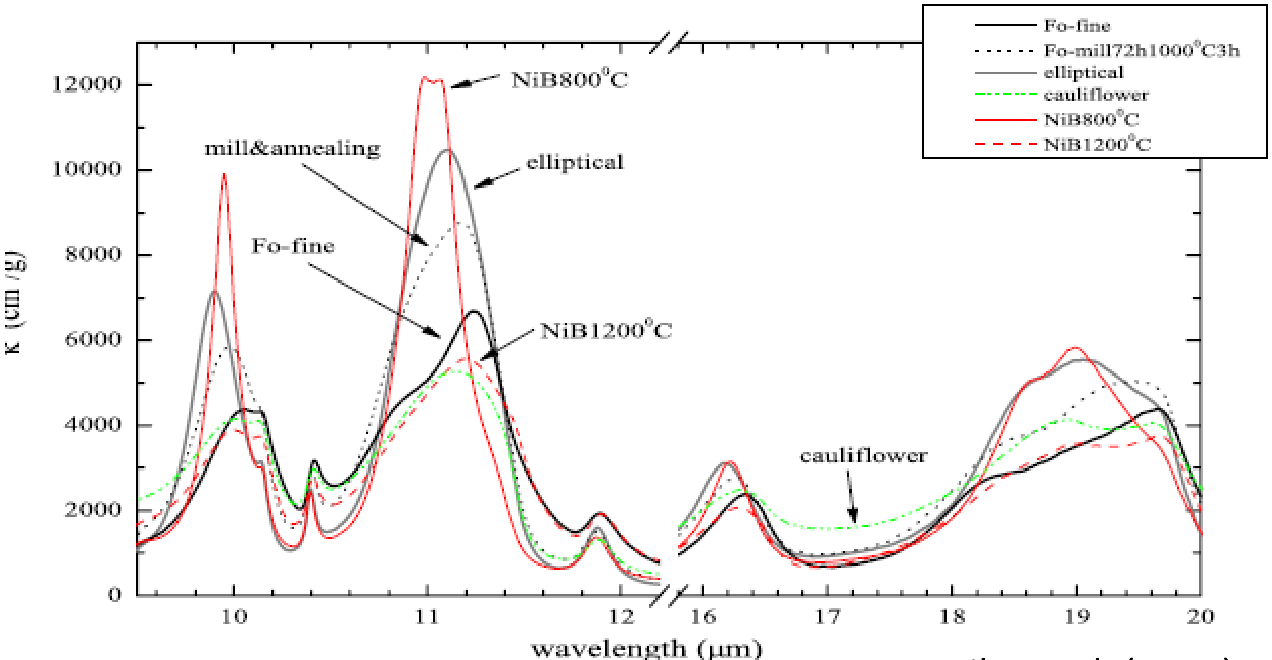
Koike et al. (2006)

Papers on grain shape effects

- Imai et al., A&A, 2009, „Shape and lattice distortion effects …“
- Tamanai et al., A&A, 2009, „Morphological effects on IR band profiles…“
- Mutschke et al., A&A, 2009, „Laboratory-based grain-shape models“
- Koike et al., ApJ, 2010, „Effects of forsterite grain shape on IR spectra“

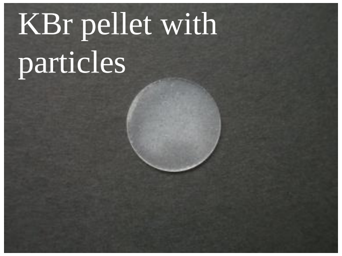


(b) annealing at 800 °C 24h



Koike et al. (2010)

Two ways for comparison spectra



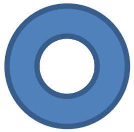
Measured:

- Spectra available for small grains (a<<λ)
- Extinction efficiency measured instead of emission, (equivalent only for a<<λ)
- Particles often embedded in solid material

Calculated:

- High computational effort for realistic grain shapes
- Simpler models prefered
  - CDE: Bohren & Huffman (1983)
  - DHS: Min et al. (2003)

Continuous Distribution of Ellipsoids



Distribution of Hollow Spheres

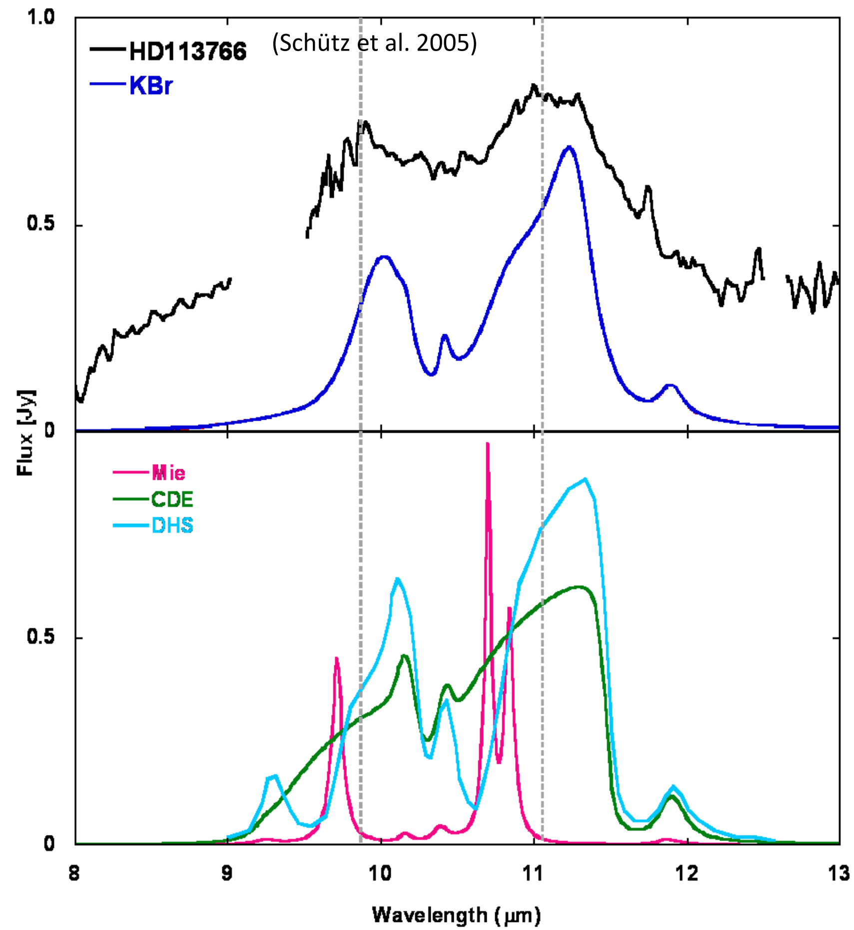
How big are the differences?

Measured spectrum (small forsterite grains)

- KBr pellet

Calculated spectra (small forsterite grains)

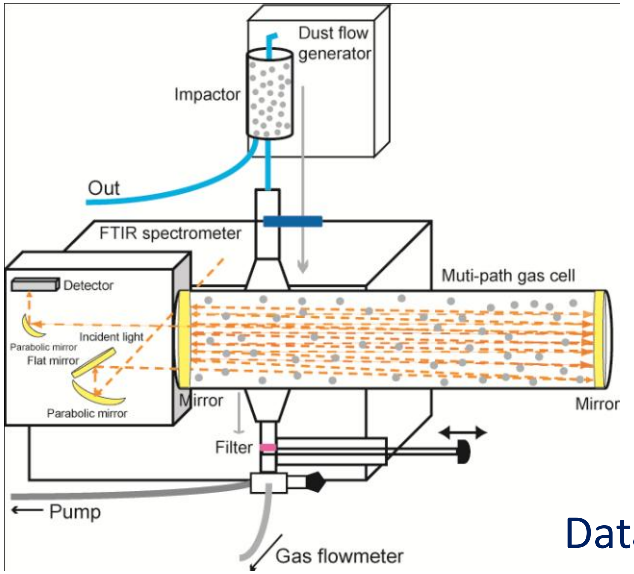
- Mie: spherical grains
- CDE: Distribution of Ellipsoids
- DHS: Distribution of Hollow Spheres

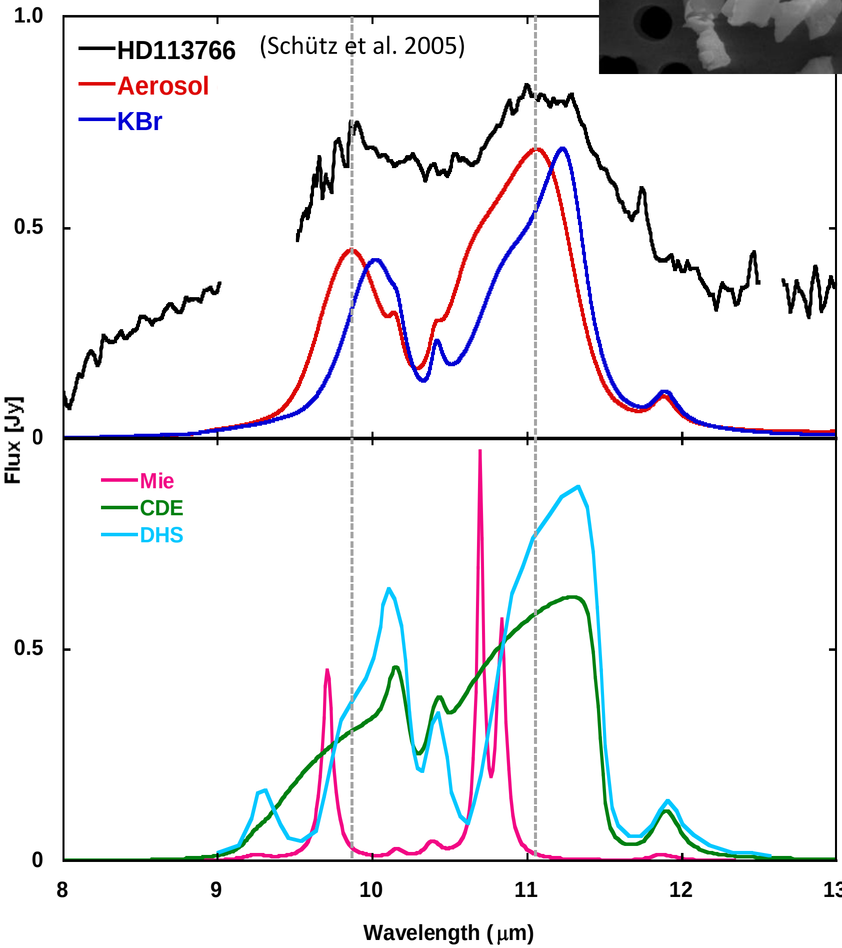


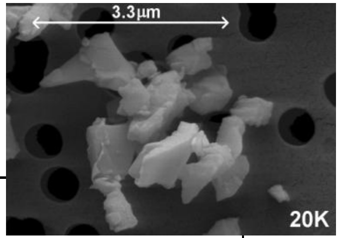
Aerosol spectroscopy

New:
- no embedding (just carrier gas)
- grain morphology analysis

Drawbacks:
- not quantitative
- still extinction measurement





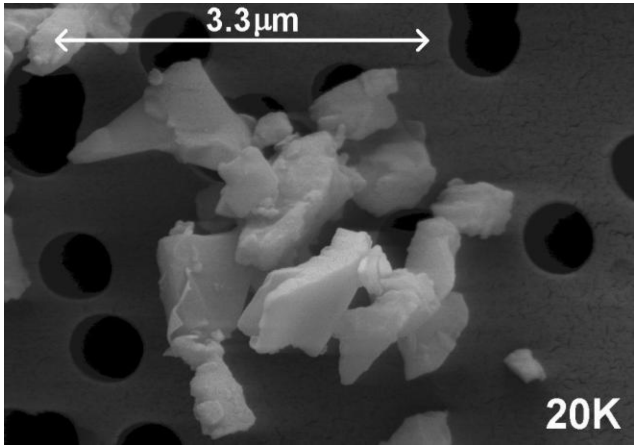


Database: http://elbe.astro.uni-jena.de

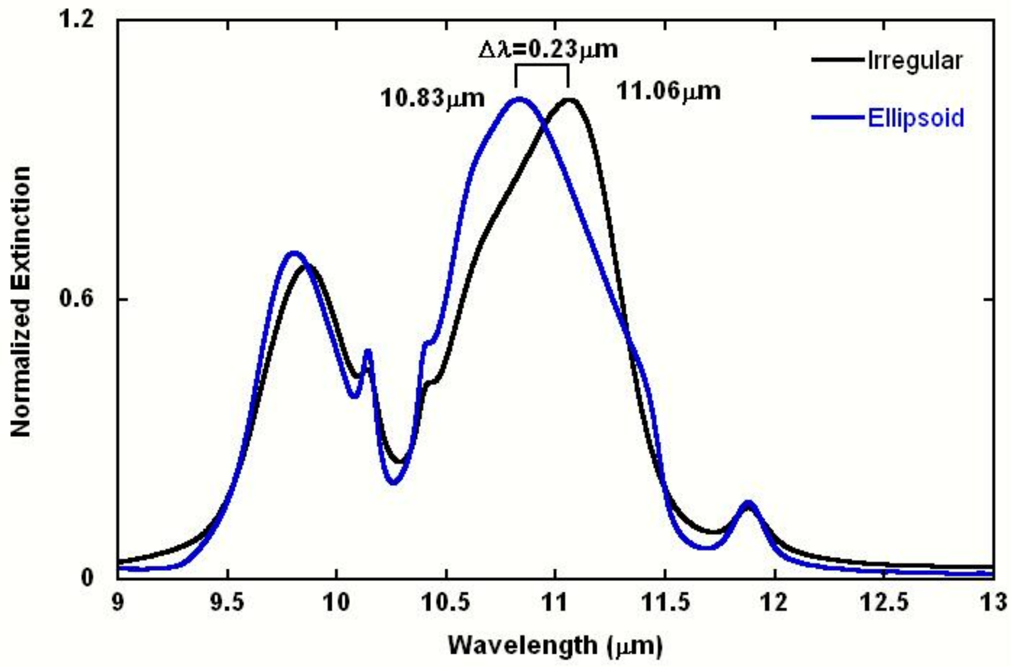
Tamanai et al. 2006

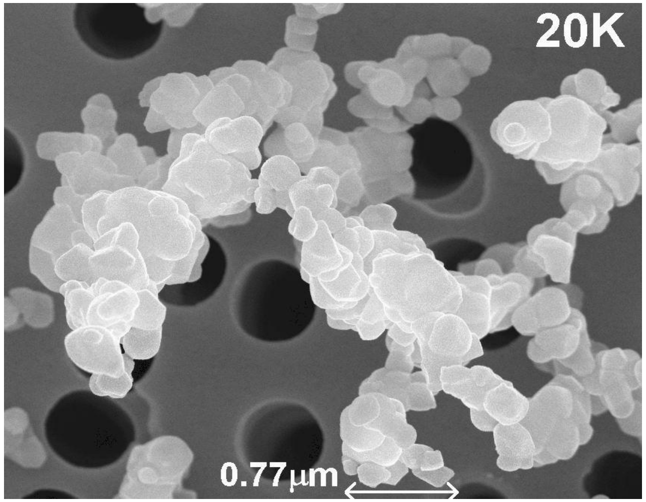
Grain shape effects in experiment

Forsterite (Mg_2SiO_4) grains with different shapes



Irregular forsterite grains



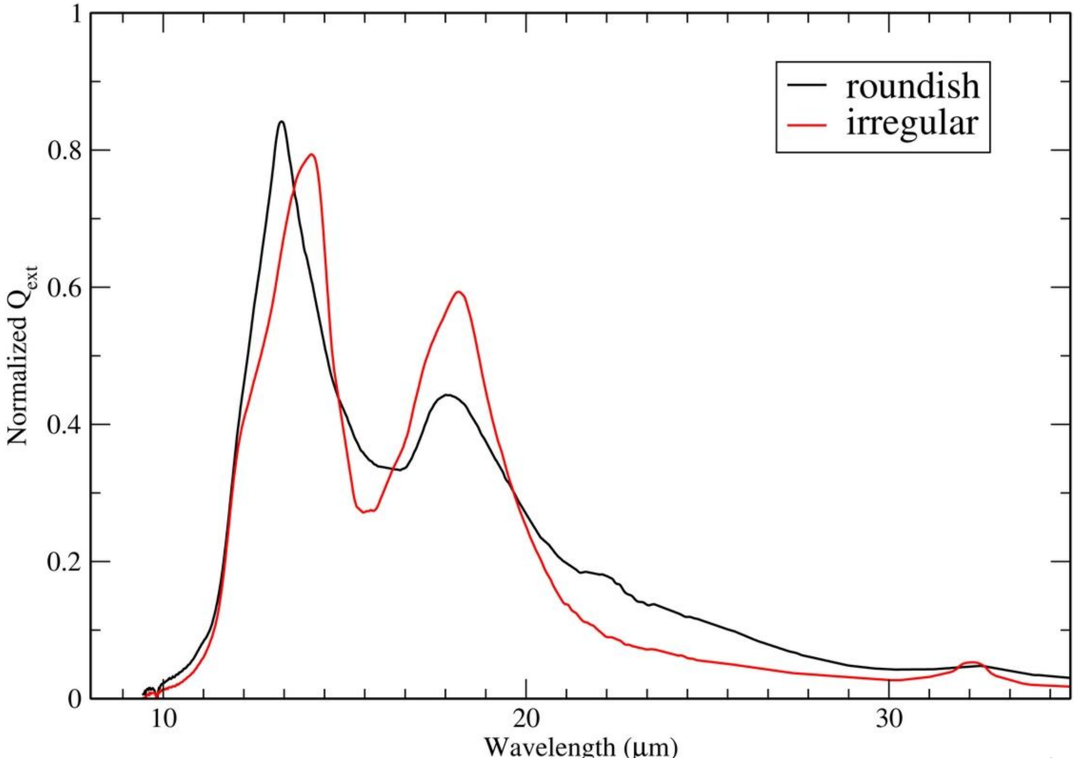


Tamanai et al. (2006)

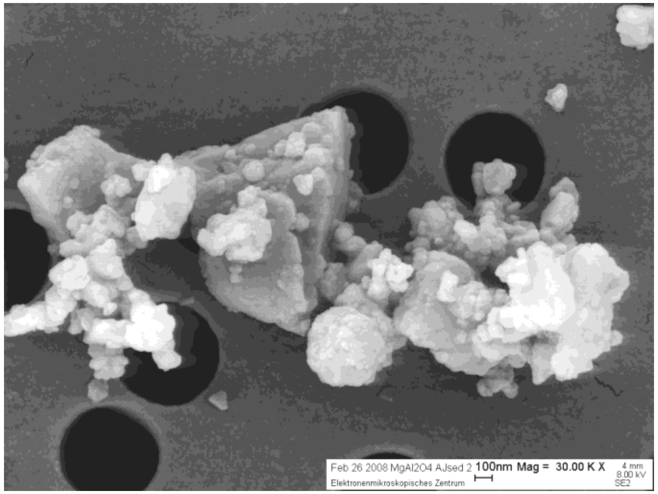
Ellipsoidal forsterite grains

Grain shape effects in experiment

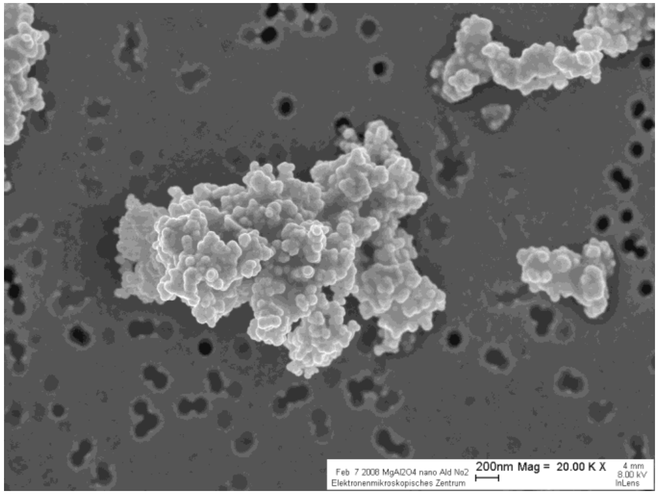
Spinel ($MgAl_2O_4$) grains with different shapes



Tamanai et al. (2009)



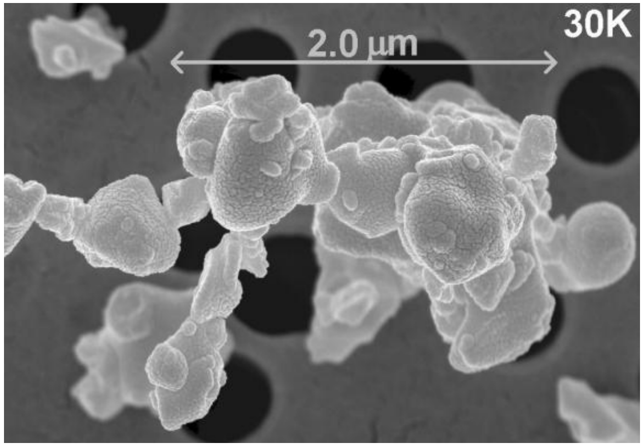
Irregular spinel grains



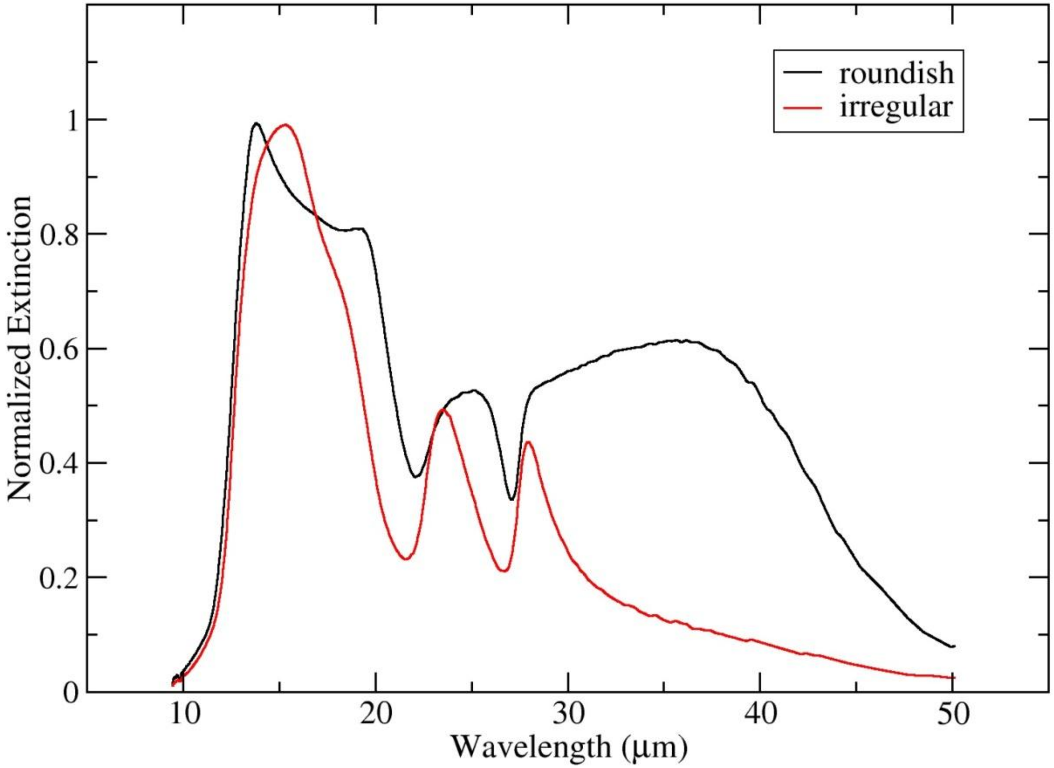
Roundish spinel grains

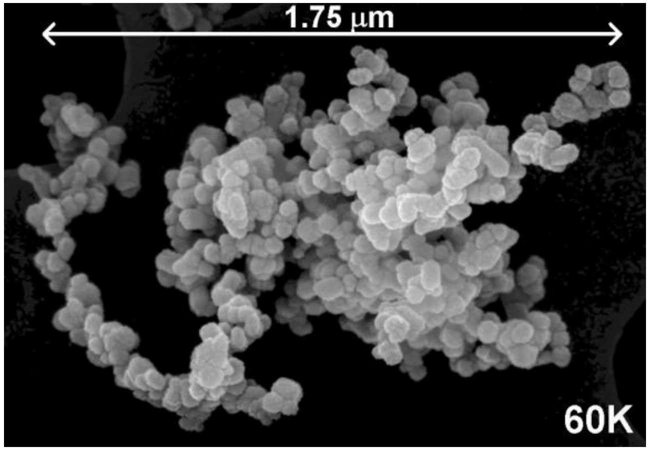
Grain shape effects in experiment

Rutile (TiO_2) grains with different shapes



Irregular rutile grains



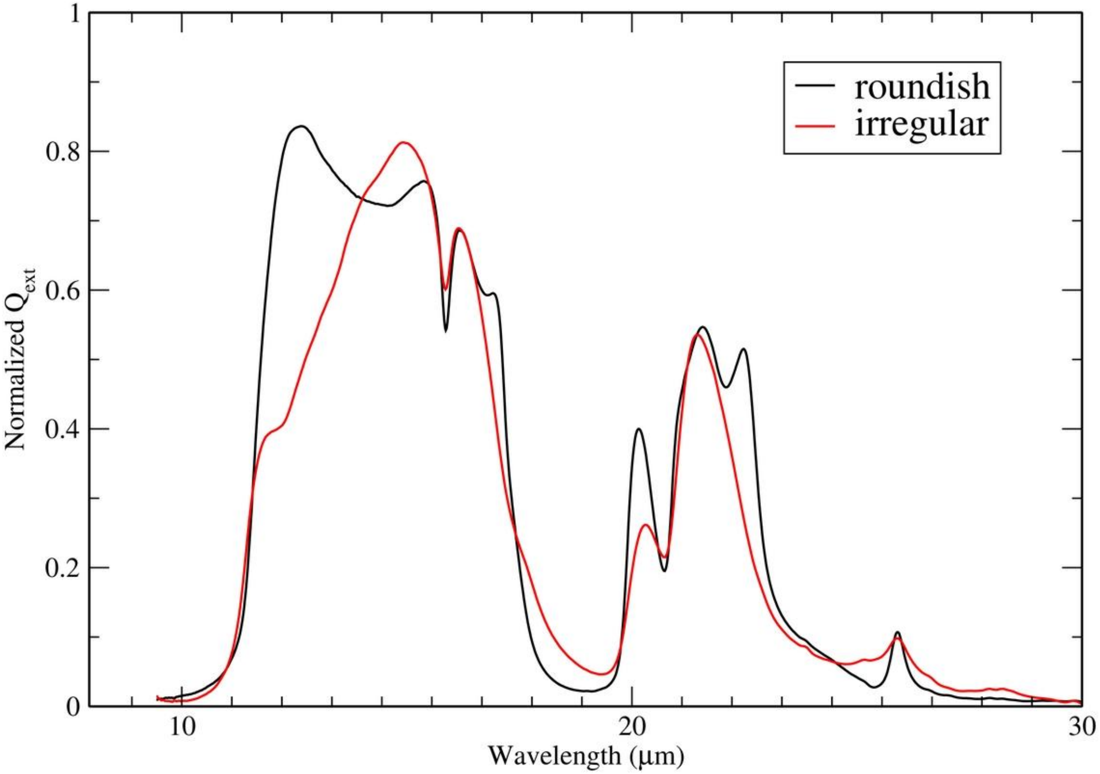


Tamanai et al. (2009)

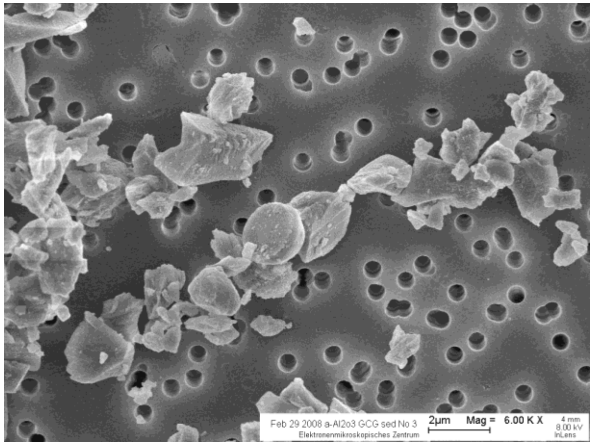
Roundish rutile grains

Grain shape effects in experiment

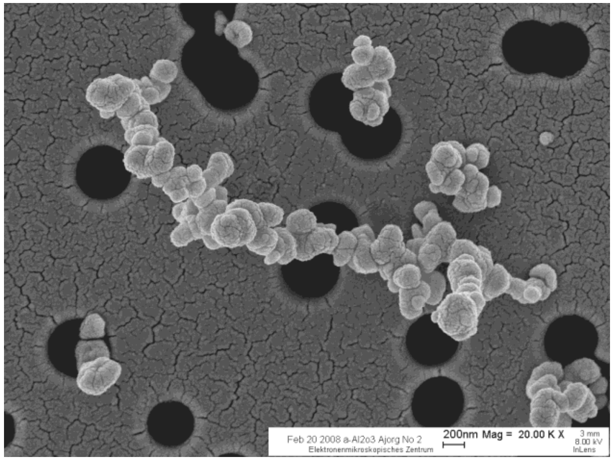
Corundum (Al_2O_3) grains with different shapes



Tamanai et al. (2009)



Irregular corundum grains



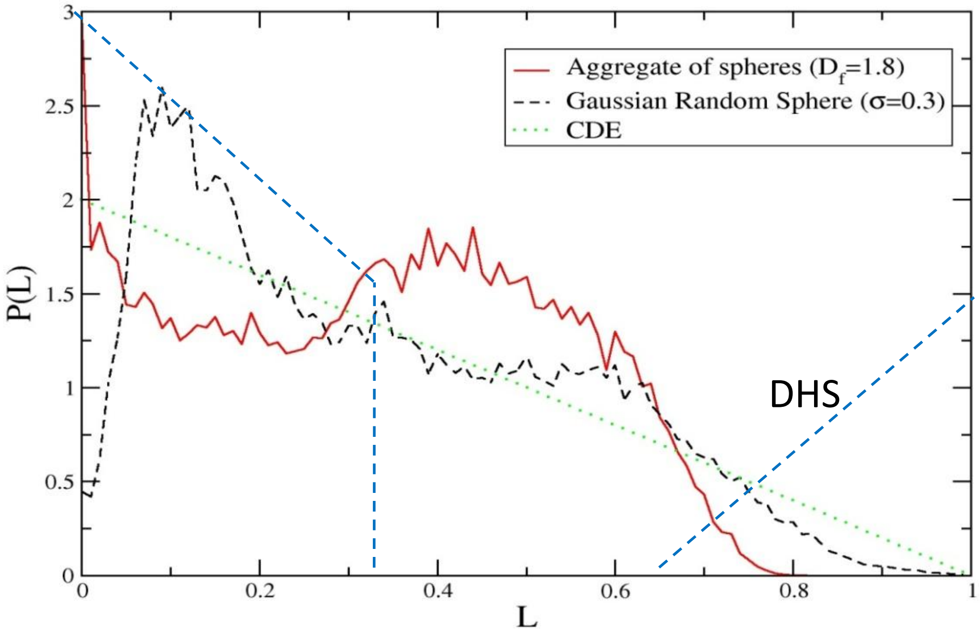
Roundish corundum grains

Theoretical description

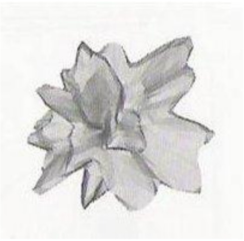
Distribution of Form Factors (DFF, Min et al. 2006):

$$\frac{< C_{ext} >}{V} = \frac{2\pi}{\lambda} * \int_0^1 \mathrm{Im} \frac{P(L)}{1/(\varepsilon - 1) + L} dL$$

(valid for small grains)



„Gaussian Random Sphere“

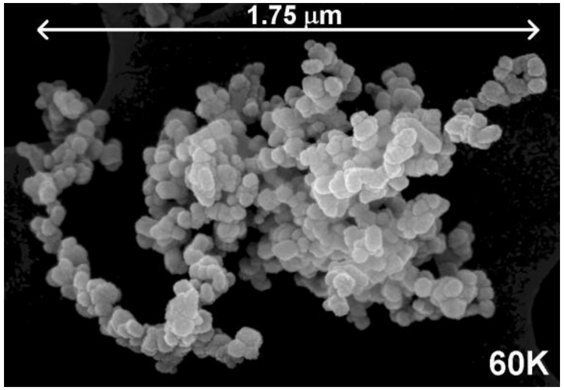


„Fractal Aggregate of Spheres“

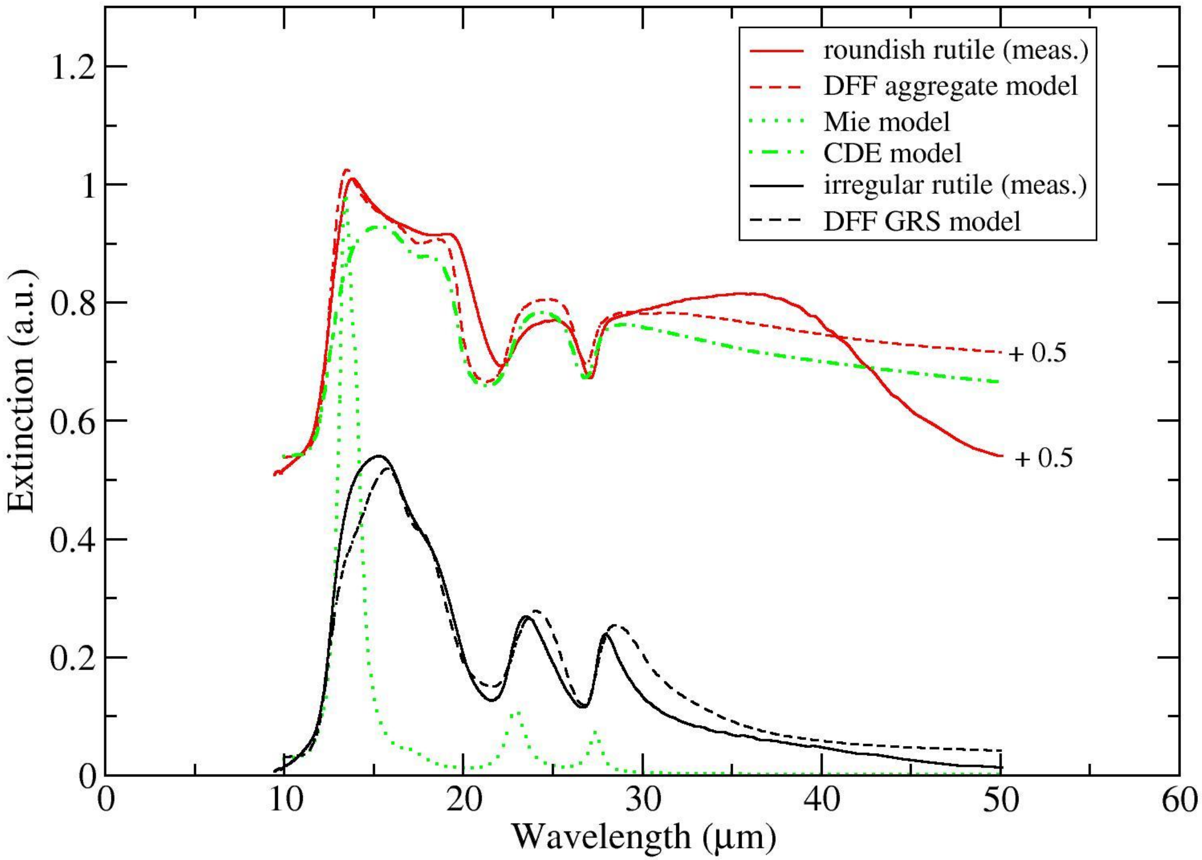
P(L) can be calculated from a discretized grain shape!

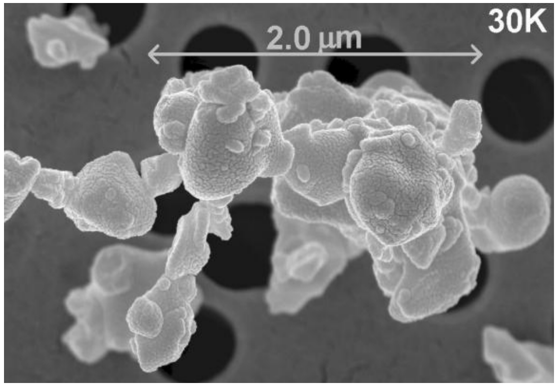
A grain of sufficiently complex structure represents also a shape distribution and vice versa! ⇒ „The statistical approach“ (Min et al. 2003)

Comparison with experimental spectra

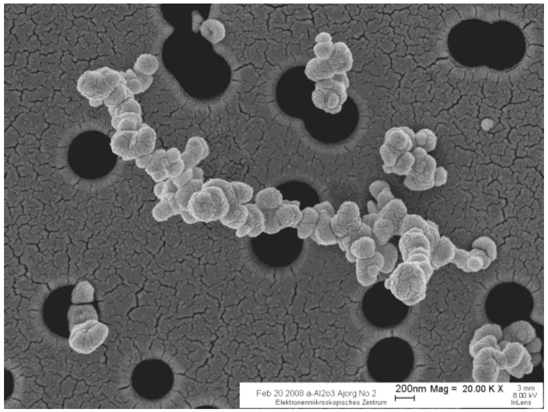


Rutile (TiO_2)





Comparison with experimental spectra

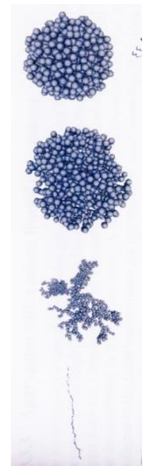


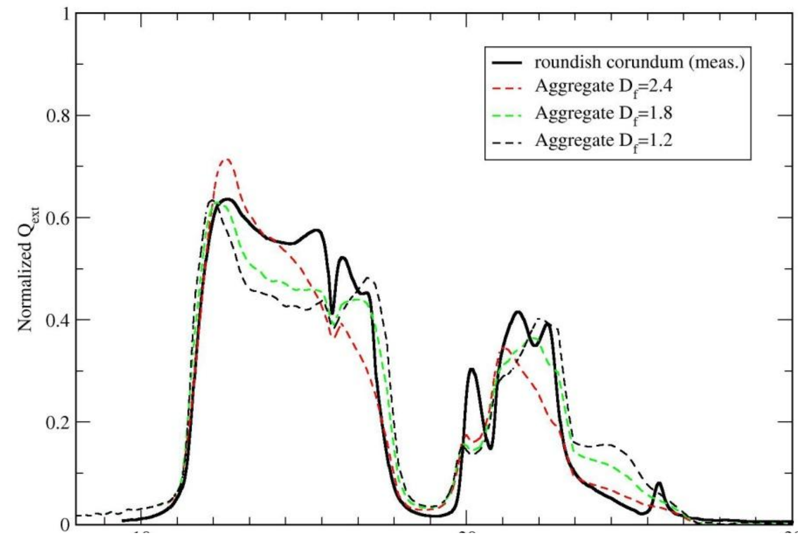
D_f=2.8

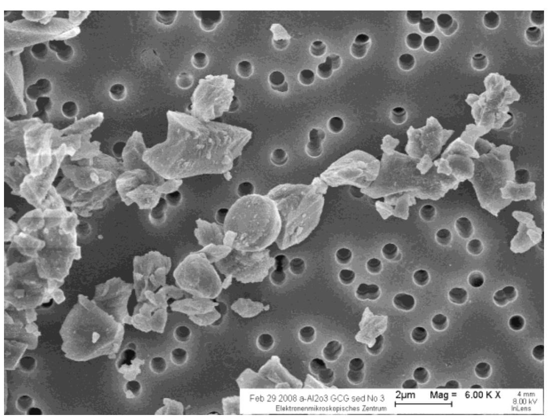
D_f=2.4

D_f=1.8

D_f=1.2





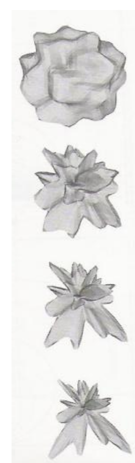


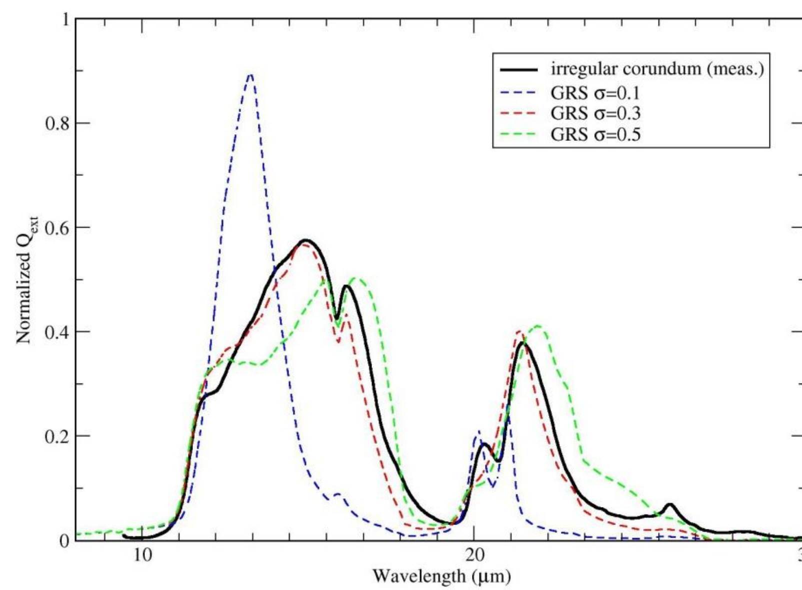
σ=0.1

σ=0.3

σ=0.5

σ=0.7



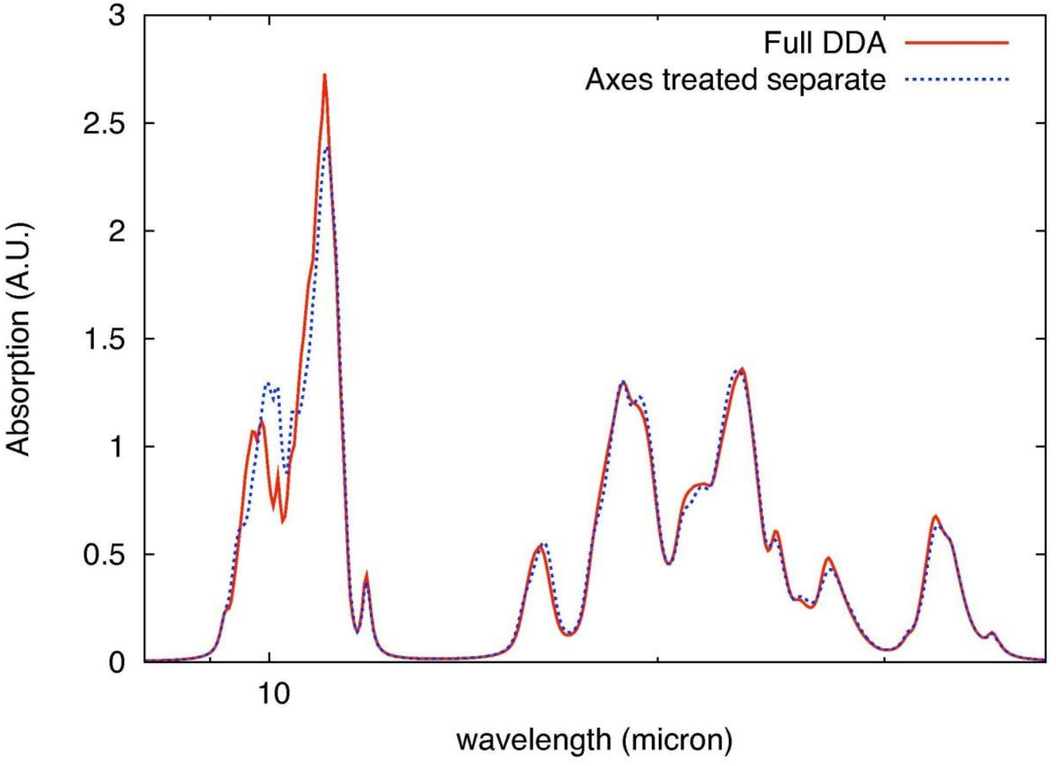


Corundum (Al_2O_3)

Mutschke et al. (2009)

Anisotropy problem

- Separate treatment of crystallographic orientations is incorrect in case of nonspherical shapes
- ⇒ Fail of simple shape distribution models (incl. CDE, DFF)
- Discrete Dipole Approximation (DDA) can take this into account

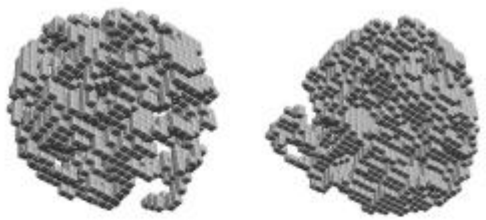


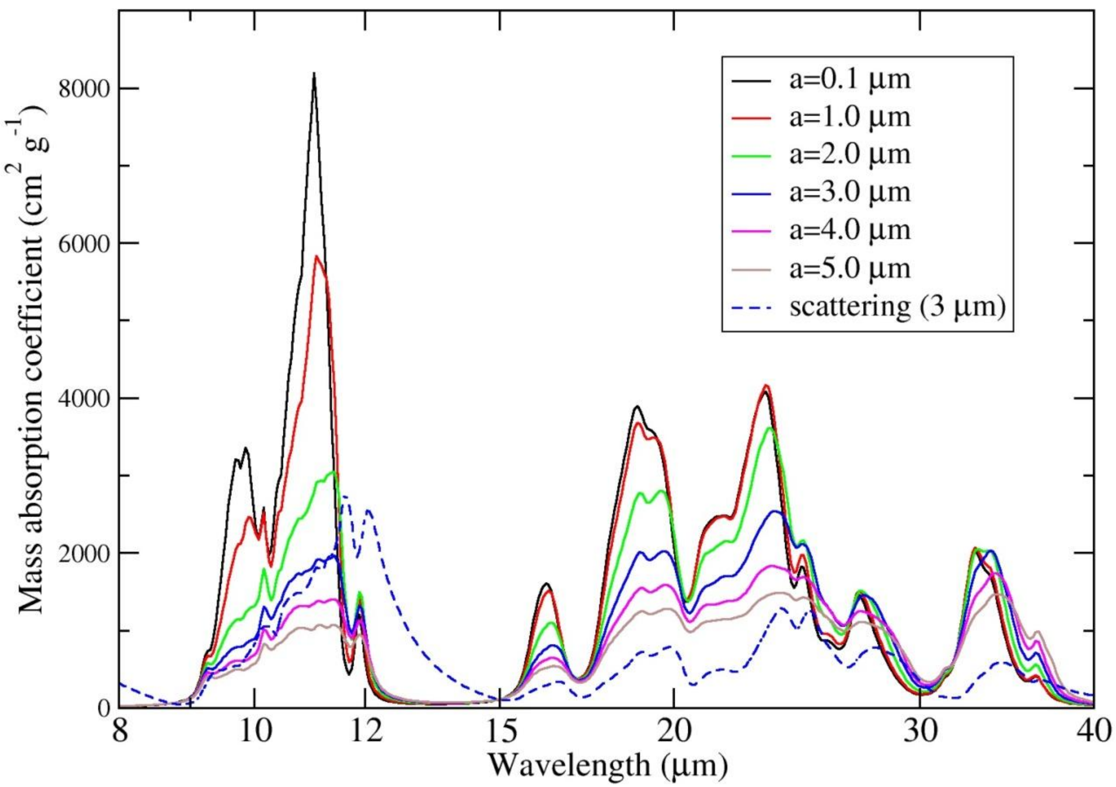
Min et al., A&A, submitted

Calculation of size-dependent spectra (using DDA)

- irregular porous grain shapes (GRF particles), averaged

- full treatment of crystal anisotropy



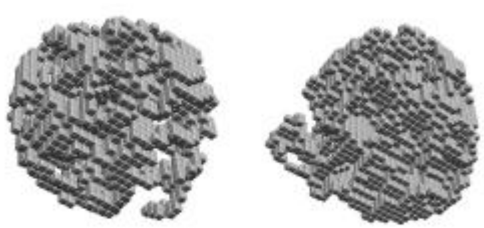


Interesting: peak shift to larger wavelength!

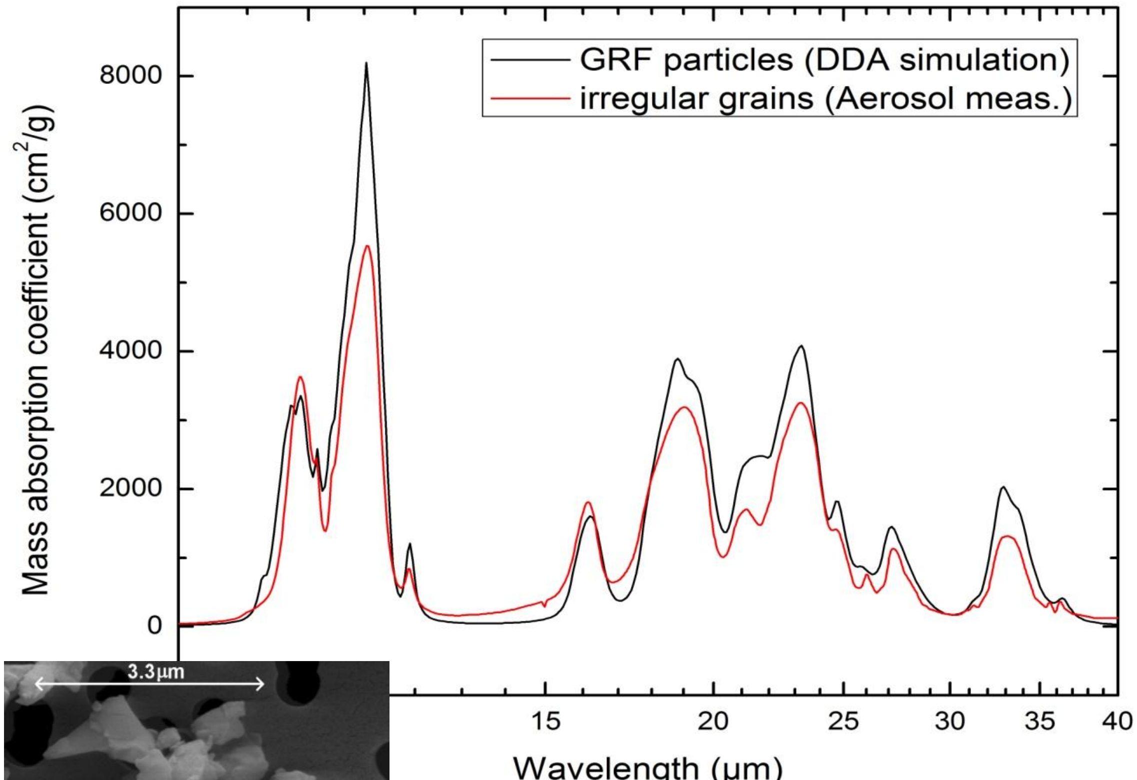
Min et al., A&A, submitted

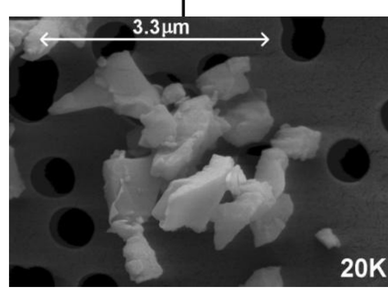
Calculation of size-dependent spectra (using DDA)

- irregular porous grain shapes (GRF particles), averaged
- full treatment of crystal anisotropy



Comparison with small grains measurements





Min et al., A&A, submitted

Summary

- Experimental spectra may be safer than simple calculated ones (as long as small grains are sufficient to consider)
- The grain-shape dependence of these can be understood in terms of shape factor distributions
- DDA model spectra - taking material anisotropy correctly into account - are coming up for larger grains