Stochastic modelling of narrowly-distributed silicon nanoparticle synthesis

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Introduction

Why model the synthesis of silicon nanoparticles?

- We learn more about the decomposition of silane into silicon
- Silicon nanoparticles have a wide range of applications

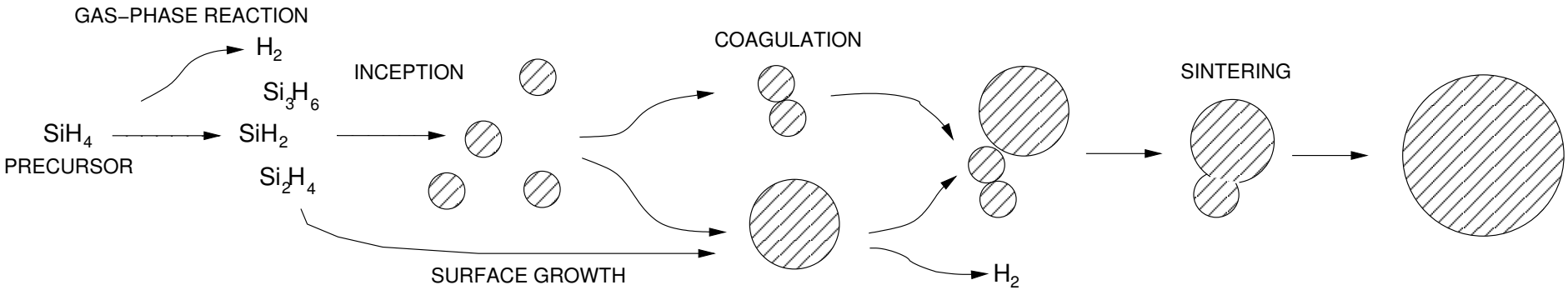
Producing nanoparticles to a controlled diameter requires an understanding of the fundamental processes controlling their formation

- How does silicon transfer from the gas- to particle-phase?
- How can we make particles of specified size and shape?

Synthesis of silicon nanoparticles

Particles are produced by the thermal decomposition of silane

- Bulk reaction: $SiH_4 \rightarrow Si + 2H_2$
- Complex inter-connected particle processes transfer silicon from the gas- to particle-phase:



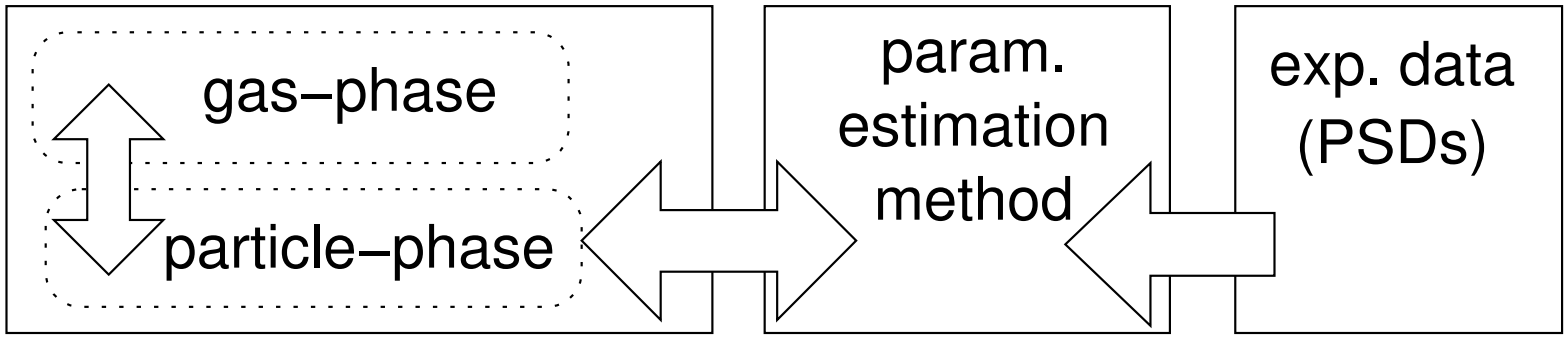
Controlling the particle size distribution (PSD) is important

- Narrow PSDs are indicative of uniform particle sizes
- Typically have geometric standard deviation (GSD) <1.10

Modelling methodology

A fully-coupled gas-phase and particle model was used

- Unknown model parameters were found using a systematic parameter estimation program
- Experimental PSDs were used for parameter estimation



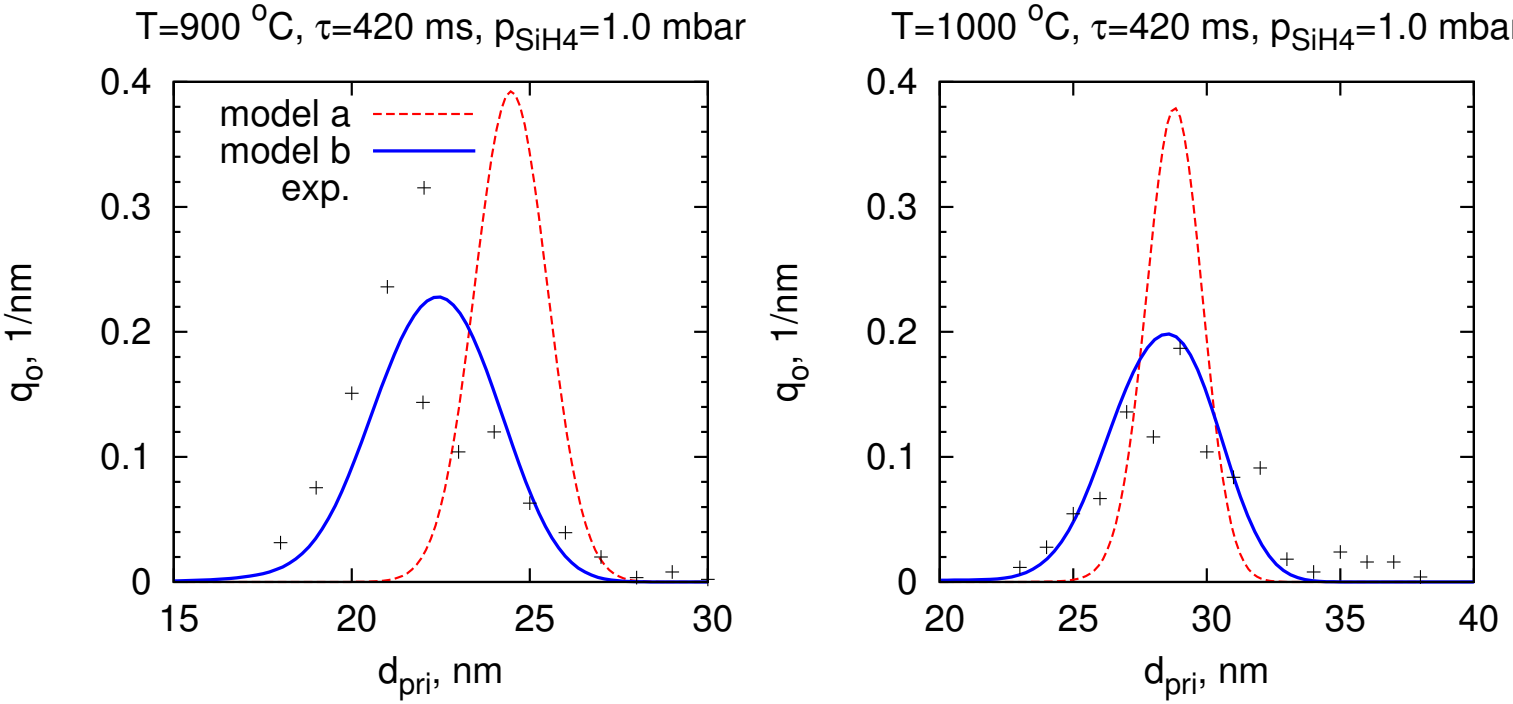
Two models were proposed

- Model A: adjust sintering parameters
- Model B: adjust gas-phase parameters

Results: PSDs

Both models gave approximate fit to the experimental data

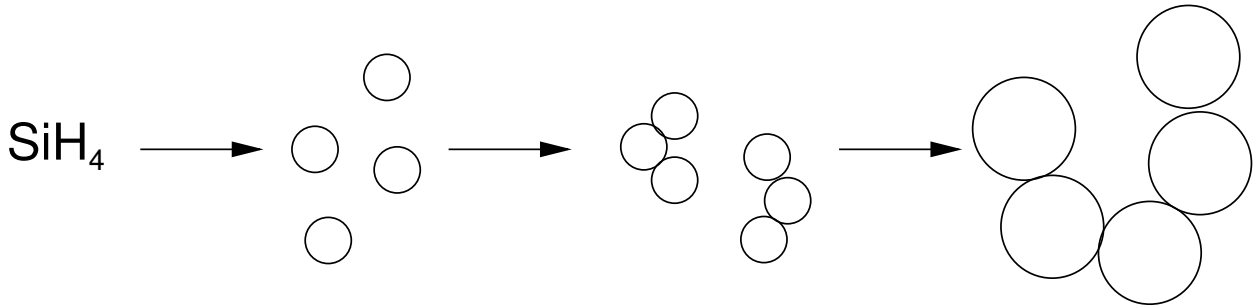
- Model B generally showed better agreement with PSD mode
- Model A's PSDs were typically too narrow



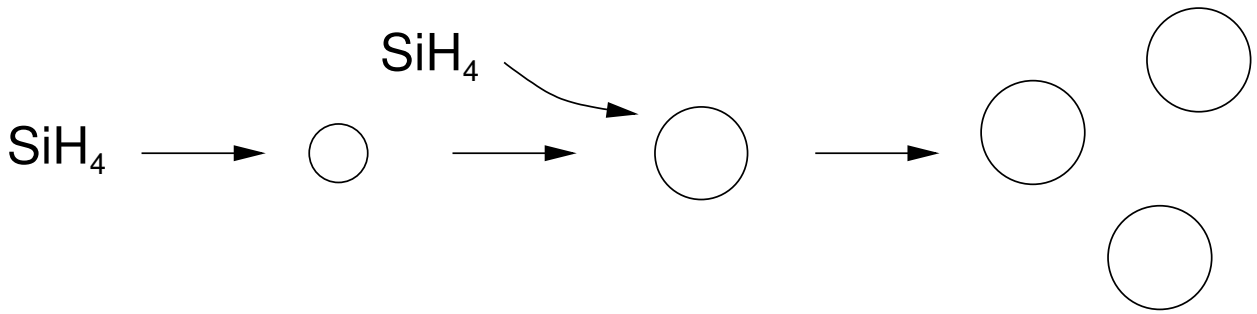
Results: Mechanisms

The models predict different mechanisms of particle formation

- Model A: coagulation and sintering form aggregates of narrowly-distributed primaries



- Model B: surface reaction suppresses coagulation forming individual spherical particles



Conclusions

- Best agreement with experimental results is obtained by adjusting the gas-phase and surface-growth rates (Model B)
- Narrowly-distributed nanoparticles can be synthesised when surface reaction is promoted and coagulation suppressed

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