# IMPROVEMENTS TO THE DESIGN OF A PARTICLE BEAM CLUSTER SOURCE FOR NANOFABRICATION

Stuart Thornton, Chris Binns and <u>Shian Gao</u> University of Leicester, Leicester, LE1 7RH, UK

### Abstract

Nanoparticle clusters often have novel properties due to the ratio of the number of atoms at their surface compared to number of atoms within their volume. This paper reports an investigation using the finite volume method to examine the flow of carrier gas and nanoparticles through a particle beam cluster machine. Numerical tests were performed with different geometries and pressures to view changes of the nanoparticle trajectory through the cluster machine. They offer an insight into the characteristic sonic/supersonic expansion of a free gas jet into a partial vacuum. The aim is to use this greater understanding to examine how the efficiency of a particle beam cluster machine can be improved.

### Introduction

Gas-phase nanoparticle synthesis involved in cluster formation and growth of gas phase nanoparticles at atmospheric pressure has been widely studied [1]. The mechanisms involved are also relevant to the formation of clusters at lower pressures. The nanoparticle sources at the University of Leicester produce particles by mixing an atomic vapour of the material required with an inert gas at much lower temperature to produce a supersaturated vapour [2]. To operate the source a cloud of metal vapour is created by heating or sputtering (see below) and mixed with an inert bath gas such as pure Helium or Argon in a primary sealed chamber with a single exit aperture (Fig. 1).

Gas-phase synthesis is more flexible and achieves better size control than any other nanoparticle production method but suffers the major disadvantage that the production rate is very low. Part of the problem is the inefficient transport of nanoparticles from the highpressure region in which they are produced to the substrate at high vacuum and this is entirely controlled by the transport at the high pressure end since throughout the rest of the source the particles form a molecular beam. The aim of this project is to model the gas flow in the high pressure region of a gas aggregation source to optimise the efficiency of transport and thus the nanoparticle flux.



**Fig. 1** A schematic layout of a typical gas aggregation source (cluster source), using a Knudsen cell for sample material heating.

#### **Models and Simulation Procedures**

Five models (A - E) were constructed to examine the role of geometry on the gas and nanoparticle flow. The geometry of the model developed for computer simulation is cylindrical, with the main apertures positioned symmetrically along the centre axis. The single input, along with a central aperture/nozzle (within the system) and the output of interest is positioned symmetrically along the central axis. A second output exists on the tube outer wall, between the two apertures and is perpendicular to the flow. The mesh generated for each model is 2d structured grid, developed using software Gambit [3].

The Fluent [3] software was used for the flow simulations. Each model was examined for a Helium gas input flow at 300 Pascal. Further tests to examine the effect of pressure changes were performed on model B, between the ranges of 100 to 600 Pascal input pressure. To further examine the gas flow and its effect on the transport of small nanoparticles, the discrete particle option was used. This allows the user to inject a second phase (with user defined properties) into the system. The discrete particles are injected as a second phase from faces in free space, set at specific geometry positions within the models. As sub-micron discrete particles flows are considered, the following options were activated in the Fluent solver options: Brownian motion, Saffman force and Drag slip. Second Order Upwind was chosen from the solution parameters, and the segregated pressure based solution SIMPLEC is used for solving the coupled system of continuity and momentum equations.





**Fig. 2** Velocity contours for Model A, at a pressure input of 300 Pascal, showing velocity magnitude and velocity vectors in the nozzle and second aperture regions.

Fig. 2 shows that the gas jet expands on leaving the nozzle and reaches the maximum velocity by the first sample position. The velocity then slowly decreases as it travels towards the skimmer, before a rapid decrease when the gas jet passes through the throat (the smallest diameter position) of the skimmer aperture. There is a second, smaller increase in velocity as the remaining gas jet exits the skimmer throat.

Fig. 3 shows the mass flow at 300K and 77K for the various aperture combinations (models A - E). It is evident that for every model, cooling the first aperture to liquid nitrogen temperatures has a dramatic increase on the mass flow in and out of the system, along the central apertures. The performance of Model E shows very high efficiency, even when used

at room temperature. It has the highest efficiency of axial output to input of 91%, (when the first nozzle is un-cooled), and when cooled the mass flow is significantly higher than for the other systems.



**Fig. 3** Mass flow of Helium gas dependent on model type (model A - E)) and the temperature (K) of the first aperture.

## Conclusions

Five different geometry models under different operation pressures and temperatures have been successfully simulated using the finite volume method, and the most efficient parameter combinations have been obtained. Further investigations of particle traces and pathlines under different operation pressures and temperatures, the temperature effects from the crucible, etc have also been conducted and will be reported in detail in the full paper. It is noticeable that the different sizes of nanoparticle can be recognised on the curved trajectory (caused by the rapid change of direction), which can be used to create focussing nozzles to concentrate nanoparticles along the main gas jet axis [4].

### References

1. Frielander S K 2000 Smoke, Dust and Haze (New York: Oxford University Press)

2. S. H Baker, S. C. Thornton, K. W. Edmonds, M. J. Maher, C. Norris, C. Binns Rev.Sci. Instrum. Vol 71. P 3178 (2000)

3. FLUENT 6.3 User's guide (2008)

4. Peng Liu, paul Ziemann, David B. Kittleson and Peter McMurray, Aerosol Science and Technology 22:314-324.