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The 130 samples from Sterkfontein and Coopers Caves which I shipped back to Switzerland in September 2005 arrived safe and sound. A large percentage of the samples were from bore-hole cores, drilled by Tim Partridge in 1989. In order to preserve the integrity of the cores, which have been heavily sampled already, I cut all the bore-hole samples in half. These have been catalogued, and half of each sample packed away. It is my intention that these halves are returned to South Africa at the end of the project, and repacked with the remaining bore holes.

As an initial step, all the samples were exposed in a Beta Scanner machine, to access background levels of Uranium. This is an important pre-screening step, as without high enough Uranium levels, the dating techniques cannot be successful. This is a time consuming exercise, as the samples require exposure times of at least 4 weeks, and optimally 6 weeks.

Once Uranium rich layers are identified, samples can be prepared for dating. This involves extensive lab work, and can take up to five days to prepare ten samples. Samples are then measured on the MC-ICP-MS (Multi-Collector Inductively Coupled Mass Spectrometer). Data produced is then analysed and eventually ages can be calculated. The whole process, from the pre-screening to age calculations, is still experimental. The development and refinement of these techniques is an aspect of my PhD. I repeated this process four times between November 2005 and June 2006. Access to the MC-ICP-MS is a major limiting factor, the machine is busy and we are a big lab, so a week of measuring time every four to five weeks is standard.

Despite all this, we have produced sufficient data from two Sterkfontein samples and one Coopers sample to calculate some new ages. The Sterkfontein ages are intriguing as they are substantially younger than the ages produced by different techniques. However, these are early days, and a re-assessment of the stratigraphy at Sterkfontein is included in this project and may go a long way to reconciling the apparently contradictory ages. The sample from Coopers Cave produced an age well within the estimated age of the site from the fossil fauna recovered, and gives us hope in our methods!

These preliminary results were presented at an INQUA workshop on Human Evolution and Climate Change in Africa in Nairobi in July, at the Goldschmidt Conference for Geochemistry in Melbourne in August and at the Palaeontological Society of South Africa's biannual meeting in Grahamstown in September. I received positive and constructive feedback at all three meetings. The Goldschmidt abstracts are published in the journal *Geochimica et Cosmochimica Acta* (volume 70, issue 18, Supplement 1). A copy is attached.

I spent about a month in September/October 2006 in South Africa doing further field work. I took a few more samples from Sterkfontein and Coopers. I also visited Swartkrans, and with the permission of Travis Pickering (no relation!) and Morris Sutton, collected a few samples for some preliminary analysis in Bern.

In 2007 new laboratory facilities will be available in the Institute for Geology at the University of Bern. With these new, ultra clean laboratories I should be able to produce better data, and calculate more precise ages. I have no plans to do any more field work, and instead need to concentrate on the laboratory work and analysis of the stratigraphy. I will also undertake some stable isotope (carbon and oxygen) analysis either at the University of Lausanne or here in Bern.

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Goldschmidt Conference Abstracts 2006

## Application of molecular dynamics simulations to the study of the growth of minerals from solution

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The nucleation and growth of crystals from supersaturated solution is one of the fundamental processes in chemistry. In many cases, the morphology and chemico-physical properties of a mineral can be determined by the growth conditions such as solvent, supersaturation, temperature, pressure and impurities. Unfortunately, the growth process occurs on a very thin layer at the crystal-solution interface and is rather difficult to characterize its atomistic details with the standard spectroscopic techniques.

A giant leap forward has been made two decades ago with the introduction of atomic force microscopy (AFM) that allows the real-time study of the growth process on the nanometer scale. A natural complement to this technique is molecular modeling that can be used for the interpretation of the AFM images in term of surface structure and energetic. The molecular dynamics approach is of particular interest in this respect as it allows to take fully into account the influence of entropy and solvation on the growth kinetics. In this presentation, the latest applications of molecular dynamics simulations to the study of minerals growing from solution will be reviewed and some examples will be discussed in detail to illustrate the advantages and disadvantages of this method

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## U-Pb dating of speleothems from Sterkfontein Cave, South Africa

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The absolute dating of the South African hominid bearing caves remains an outstanding issue in Palaeoanthropology. Biostratigraphic age constraints and cosmogenic isotope burial dating indicate the breccia deposits of Sterkfontein Cave are between 1 and 4 Ma. Thus speleothem material preserved at Sterkfontein is too old to date by U-Th. U-Pb dating of speleothems is possible and has been undertaken on material as young as 200 ka (Richards et al., 1998) but is a challenging task. We have adapted the method of the pioneering work of (Walker, 2005). Without modelled or measured initial  $^{234}\text{U}/^{238}\text{U}$  ratios only maximum ages can be obtained. We model initial conditions, i.e. excess initial  $^{234}\text{U}$  and depleted  $^{230}\text{Th}$ .

Samples are pre-screened using  $\beta$ -scanner imaging to identify U-rich layers. Initial MC-ICP-MS results indicate that relatively U-rich layers can exist near the base of flowstones, with U concentrations of between 0.1 and 2.4 ppm. Strong initial ( $^{234}\text{U}/^{238}\text{U}$ ) disequilibrium is found for samples younger than 2.5 Ma. Both high U and large initial  $^{234}\text{U}$  excess may result from slow weathering of bedrock, without leaching, in the arid phase preceding conditions conducive to flowstone formation.

[Pb] ranges between 20–200 ppb and is highly heterogeneous. Small scale (~cm spaced) sampling of U-rich speleothem layers provides a range of U-Pb ratios. Using MC-ICP-MS in static mode, with  $^{204}\text{Pb}$  in an electron multiplier, gives relative precision on 206/204 better than 0.13%. Thus  $^{204}\text{Pb}$  can be used as a reference for isochrons.

A number of problems remain: discrepancies between ages obtained by different dating methods, poor stratigraphic control of the breccias at Sterkfontein and estimates of initial  $^{234}\text{U}/^{238}\text{U}$  values for samples >3 Ma. Efforts to constrain the latter using O and C isotopes as proxies are underway.

### References

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