# Exchange Visit to Tübingen University
# Report

**Project Title:** Numerical modelling of air bubbles in ice - insight from partially molten rocks

**Visit Dates:** 7.05 – 03.06.2011, 4 weeks

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## Scientific Background and the Purpose of the Visit

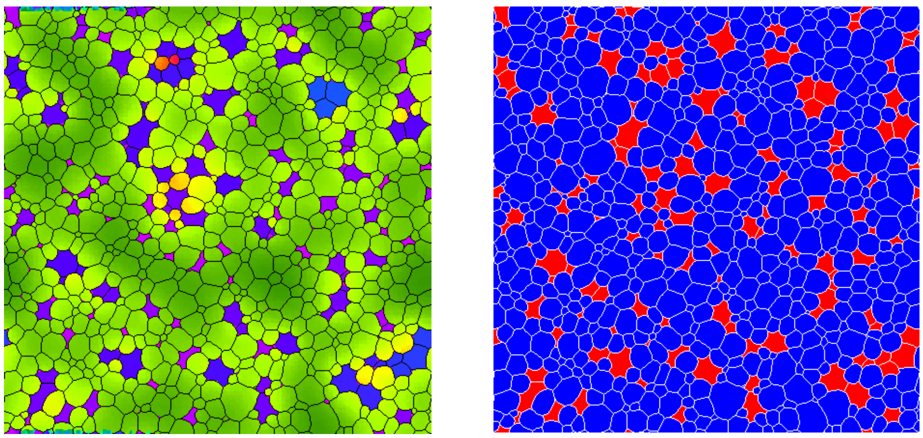
The chemical and isotopic composition of air bubbles enclosed in ice is a primary source of information on the earth's climatic record and environmental conditions. Polar ice is, however, not static, but a dynamically evolving material.

The trace element and isotopic compositions of air/gas is not constant once it is enclosed by snow. As long as air bubbles are connected, interaction between air/gas from different levels is possible. Several processes such as diffusion, thermal diffusion and gravitational settling may cause measurable shifts in isotopic composition. Once air is fully entrapped, communication between individual bubbles is strongly reduced, as it would need to involve diffusion through solid grains or along grain boundaries.

However, at present there is not enough knowledge as to which extent recrystallization and grain growth may influence interaction and exchange of isotopes and trace elements/gases. In order to investigate recrystallization and related processes, ELLE software may be used. Partially molten rocks of Earth crust and mantle show an analogous system where melt in small pockets (analogue to air bubble) interacts with surrounding mineral grains (analogue to ice crystals). As the researcher has a previous experience on working with partially molten systems the exchange visit was mainly aimed to apply this geochemical expertise and to discuss how chemical and isotopic exchange can be incorporated into the ELLE code for further simulation of polar ice microstructures. The microstructure development code is presently being developed at the host institution in Tübingen, Germany.

## Main Research and Results

J. Roessiger and P. Bons have developed the ELLE code to simulate recrystallization of ice in the presence of air bubbles. This code allows the simulations of multiple, coupled processes that act on a microstructure of ice. In this approach the microstructure is not parameterised, but actually mapped on the grain-size scale. It has become evident that during static grain growth in the presence of air bubbles, these air bubbles may shift their position and coalesce to form bigger bubbles. If air bubbles would remain static, all exchange between the two phases has to occur by diffusion. Active migration of the phase boundaries would greatly enhance the exchange between the two phases. This would apply to exchange between ice and air during firn and ice compaction. This has a major influence on the air/gas bubble chemical characteristics as observed ice core.



*Results of first simulations of diffusion in a two-phase system, showing phase distribution (right) and distribution of the concentration of a trace element (left).*

During the exchange visit, ideas were developed and discussed on how to incorporate trace element/isotope chemistry and diffusion into the existing numerical model. The basic code for trace-element and isotopic exchange between two phases with very different diffusivities and fractionation effects was implemented in ELLE. In collaboration between Tallinn and Tübingen, this still very basic code will be further developed to address specific cases in polar ice microstructure, where a multitude of processes can be recognized that affect the trace element and isotopic signature of ice/gas bubble during compaction and recrystallization. A significant step forward was made to create a combined numerical code for the simulation of micro-textural and (micro)chemical evolution of the polar ice, which in turn may facilitate the interpretation of a complex climatic/environmental signals of the ice core.

The collaboration with Tübingen University will continue in the future on the topic of ice-air bubble recrystallization and interaction. As the Estonian geoscientists at the Tallinn University of Technology have been involved in polar studies and paleoclimatology for several decades, this may be a new direction where a classical approach of ice core studies will be supported by present innovative approach of microstructural and chemical modelling. Using ELLE software, many new aspects of ice core studies can be tackled. Based on the work done during the exchange visit and forthcoming studies, a joint publication is planned to be published in a peer-reviewed magazine.

As the aim of Micro-DICE is to gain better understanding of the behaviour of ice considering the role of the microstructure and chemical exchange during a wide range of processes, the present project may have an important impact for development of knowledge on the ice core signal interpretations.

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