Comparative Analysis of Experimental and Computational Models for SIC Crystallization Using SEM-EDS Techniques

NIC LITZA[1], MIKI NAKAJIMA[1,2], SEAN O'NEILL[3], GREG MADEJSKI[3], ETHAN LUTA[4], XINYAO ZHOU[2]

[1]Department of Earth and Environmental Sciences, University of Rochester; [2]Department of Physics and Astronomy, University of Rochester; [3]Integrated Nanosystems Center, University of Rochester; [4]University of Rochester Medical School

INTRODUCTION TO SUDBURY

- The Sudbury Basin is a 1.849 billion year-old impact crater located in Sudbury, Ontario, CA[1] caused by a bolide 10 - 15 km in diameter[2]

- The original diameter of the crater is estimated at 250 km[3], reduced to ~65 km (along the semi-major axis) due to tectonic processes[4]

- Sudbury Igneous Complex (SIC) is the largest and best-preserved impact melt sheet[5]

MOTIVATION

- Hadean impacts may have played a critical role in the lack of preservation of Earth's earliest crust[6]. The role of the Hadean crust formation via this mechanism is poorly understood due to a lack of samples, SIC is a principle analogue[6]

- SIC likely formed by fractional crystallization of impact-induced melt[7], can be an important natural laboratory to study how rocks and minerals record the impact process

- Details of the crystallization process are not well constrained!

- Goal of this project is to determine the starting composition of the SIC, create a sample with this composition in a lab, apply high pressure-temperature (P-T) conditions to the sample and observe the present phases with a scanning electron microscope (SEM)

- Results are compared to simulations with alphaMELTS2

Fig. 1a. Parkin Offset Dyke located in the North Range of Sudbury. MELTS Simulations of this project used data of Offset Dykes in the South Range.

Fig. 1b. Shatter cones on the south side of Ramsey Lake. The presence of shatter cones was integral in proving the Sudbury Basin was caused by an impactor, rather than by natural geological processes.

alphaMELTS2

- alphaMELTS2 is a software designed to facilitate thermodynamic modeling of phase equilibria within magmatic systems[10][11]

- rhyolite-MELTS (v 1.1.0) can be used to simulate crystallization of magma bodies. We use this algorithm of alphaMELTS2 to constrain conditions of melt sheet crystallization (pressure, composition) based on observed SIC chemistry and mineralogy

- The starting bulk composition[9] is an average of the composition of the quartz diorite (QD) and mineralised inclusion quartz diorite (MIQD) units from the Offset Dykes (OD) of the the South Range in Sudbury. These units best represents the initial composition of the SIC prior to any crystallization processes that occurred during cooling[8]

- End goal is to understand whether crystallization of the QD and MIQD composition can reproduce the observed SIC mineralogy and chemistry highlighted in fig. 3. Achieved by finding what conditions of P, T and H_2O produce the best match

Fig. 2. The lab-created Sudbury sample (left) with the graphite furnace (right), part of the apparatus that entered into the piston cylinder.

LABORATORY EXPERIMENTS

- The QD and MIQD Sudbury bulk composition was also used to make a 2 - gram anhydrous sample
- Samples were placed in a graphite capsule and graphite furnace, pressurized and heated in a piston cylinder then quenched to form a glass

- Goal is to see how this composition crystallizes as a function of temperature and compare to a suite of simulations

- Sample composition:

Oxide	SiO_2	Al_2O_3	MnO	MgO	CaO	Na_2O	K_2O	TiO_2	P_2O_5	FeO	Fe_2O_3	S
Weight%	58.7	15.2	0.1	4.5	5.9	2.9	2.0	0.8	0.1	5.4	4.0	0.4

- Experiment conditions:

Pressure (GPa)	0.5	1.0	1.0	1.0	1.0
Temperature (C)	1350	1250	1150	1050	950
Run Duration (Days)	1 Day	1 Day	2 Days	3 Days	7 Days

- Experiments were 1 GPa, different from the SIC (0.1 GPa) due to limitations of the piston cylinder

SCANNING ELECTRON MICROSCOPE

- A scanning electron microscope (SEM) was used for high-magnification imaging, all samples were sputter-coated with gold to assist in the imaging process

- SEM uses an electron beam which scans across a surface, detecting electrons that are scattered/emitted to create of the sample's surface morphology and composition

- Secondary electrons (SE) are low-energy electrons, emitted from the surface when it is bombarded by the SEM electron beam, used in this study for imaging

- EDS (Energy Dispersive Spectroscopy) is a technique that allows the identification of elements in a sample. The electron beam causes characteristic X-rays to be emitted from sample, then detected and analyzed. Used in this study for quantification

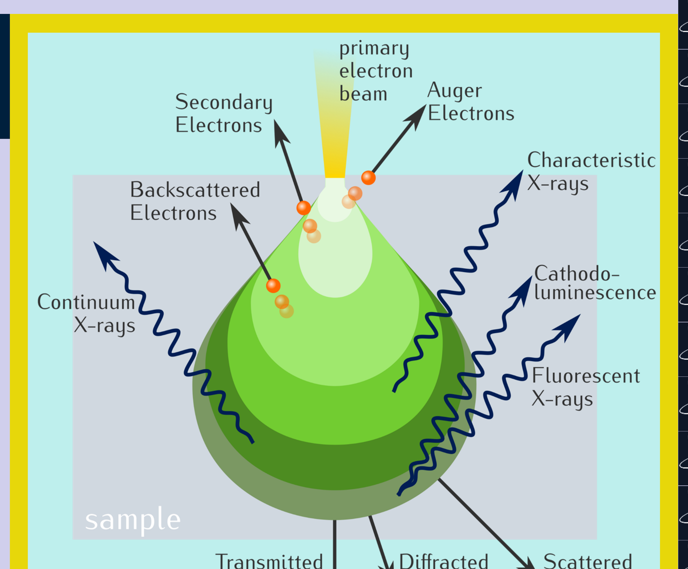
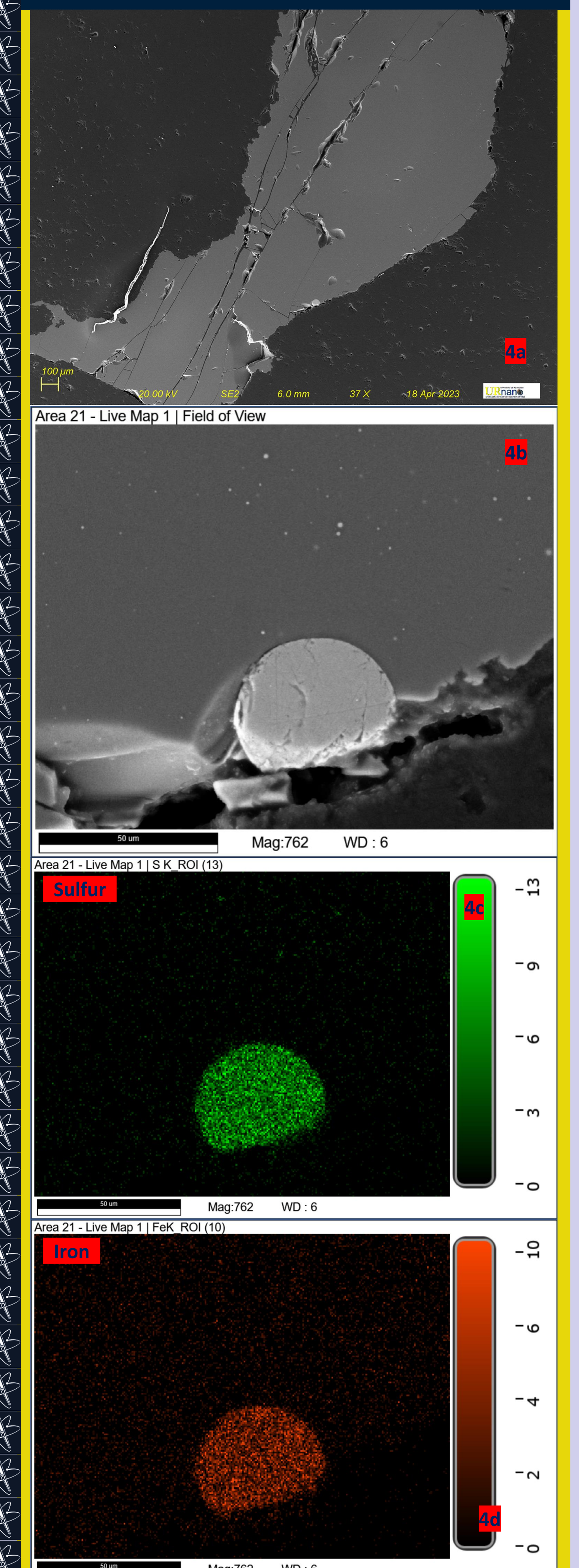
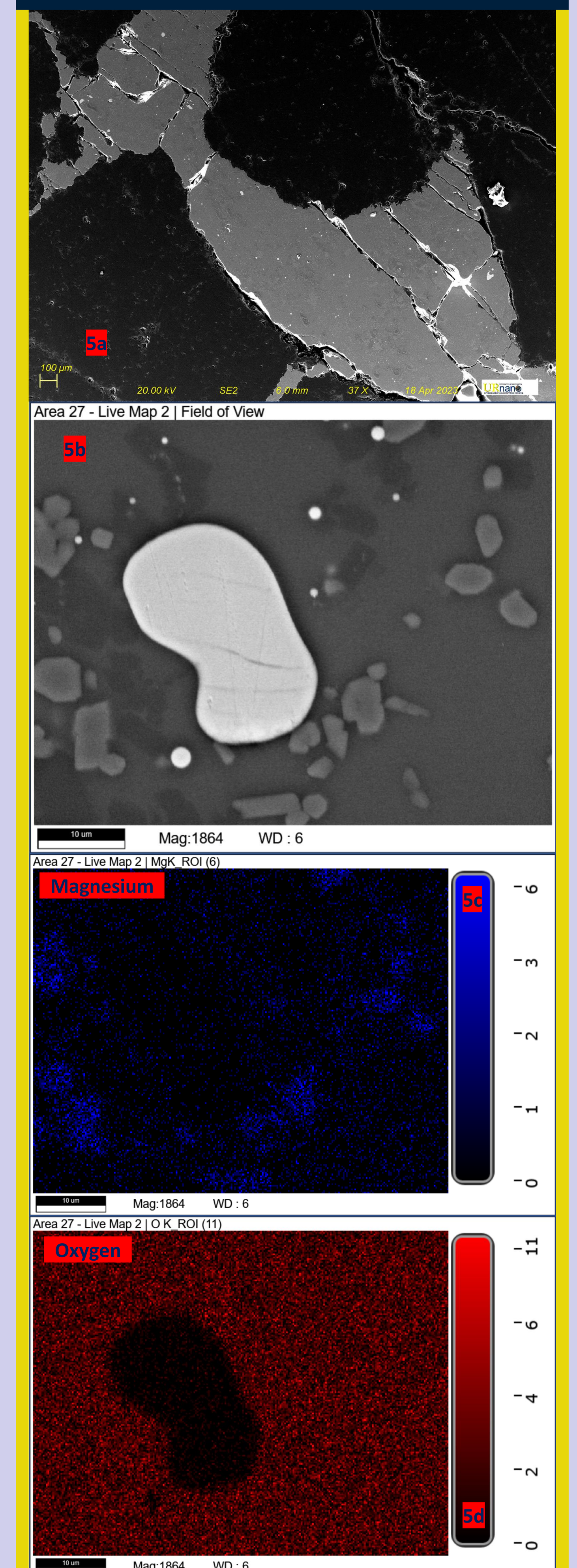


Fig. 3. SEM interaction volume of different sources. [12]

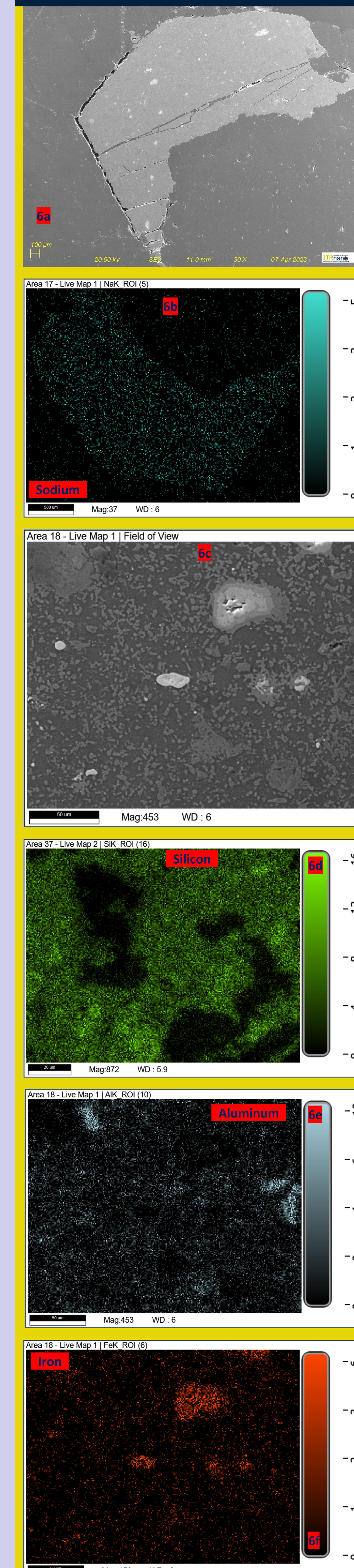
1250°C Results



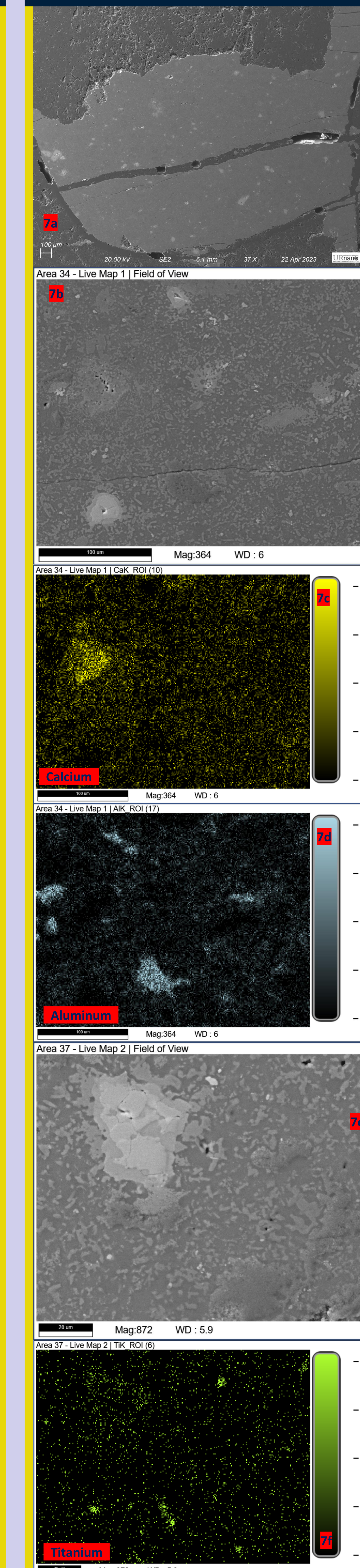
1150°C Results



1050°C Results



950°C Results



- Color maps show density of chosen element. High density of color in region implies high density of element, dark implies lack of element
- Element maps allow us to visualize the distribution of elements, which can help us identify specific minerals or mineral phases
- 1350°C sample not included as results were identical to 1250°C results

alphaMELTS2 RESULTS

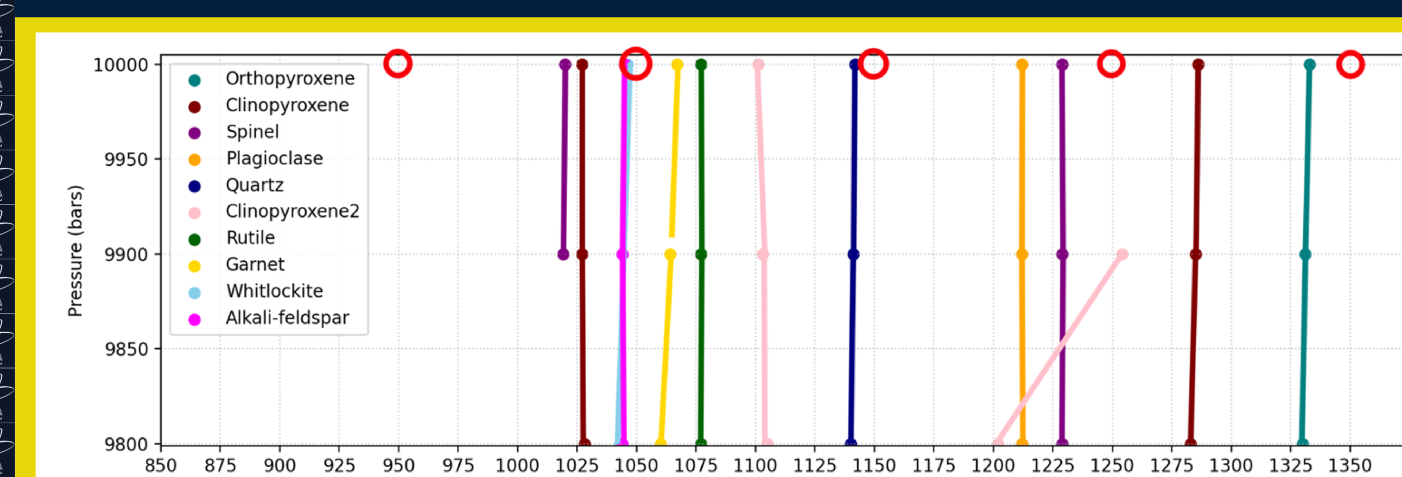


Fig. 8. alphaMELTS2 simulations with the lab bulk composition as an input. Red circles represent the point in P-T space of the laboratory experiments. 1350°C has no phase, while 950°C should have all phases.

- alphaMELTS2 simulations without water are very unstable, program is susceptible to crashing, unable to simulate to low temperatures

DISCUSSION & FUTURE WORK

- First visible phase detected with the SEM was FeS, only visible phase in 1350°C and 1250°C experiment. This is not predicted in alphaMELTS2, since S is not treated as a major element

- alphaMELTS2 is a great source for predicting phases with this bulk composition:
- - Presence of clinopyroxene and orthopyroxene by 1250°C. Neither was visible in the 1250°C sample, both are visible at lower temperatures
- - Plagioclase and spinel by 1150°C. Spinel phase prominent in the 1050°C (fig. 6f)
- - Quartz, rutile and garnet by 1050°C. Rutile is seen in the 950°C sample, highlighted in the Ti map (fig.7f). Quartz shows up at bottom of fig. 6d, garnet uncertain
- - Whitlockite and feldspar by 950°C. Whitlockite is likely seen in top left of fig. 7c, feldspar in fig. 7d

- A new sample with a more accurate Sudbury bulk composition should be made. Include Cr, Co, Ni and water to better represent the Offset Dykes. Additionally, use a better dwell process with piston cylinder

REFERENCES & ACKNOWLEDGEMENTS

Scan QR code for references

Partial funding for this research was provided by a National Science Foundation (NSF), under Grant No. EAR-2102143. Any opinions, findings, conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect those of the National Science Foundation. This work was also supported in part by the Alfred P. Sloan Foundation under grant number G202114194