**AN EVALUATION OF THE IGNEOUS CRYSTALLIZATION PROGRAMS -- MELTS, MAGPOX, AND COMAGMAT PART II: IMPORTANCE OF MAGMATIC $fO_2$** V. P. Slater (vpslater@hotmail.com), C. K. Thompson, J. Nettles, K. Milam, K. R. Stockstill, J. Cahill, M. Anand, and L. A. Taylor, Planetary Geosciences Institute, Department of Geological Sciences, University of Tennessee, Knoxville, Tennessee, 37996.

**Introduction:** This is Part II of a study to evaluate the appropriate application of magma crystallization computer models used in the geologic community. These crystallization models (MELTS, MAGPOX, and COMAGMAT) often are used without prior knowledge of the programs' strengths and weaknesses, potentially introducing error during result interpretation. Part I by Thompson et al. [this volume] examines the results produced by these computer models for three rock compositions using estimated values for magmatic $fO_2$ and 1 bar pressure. Part II of this study assesses the limitations of the programs for a range of magmatic $fO_2$ conditions.

**Methods:** The versions of the crystallization models evaluated in this study are MELTS (Mac version 5.1) [1], MAGPOX (disk version) [2], and COMAGMAT (internet version 3.3) [3]. Rock compositions are the same as those in Part I: the martian meteorite Nakhla [4], the angrite LEW 86010 [5], and the Apollo 15 basalt 15555 [6]. Approaches used to formulate each model are given in Part I of this study. Equilibrium crystallization was simulated at a pressure of 1 bar, and each rock was run at three values of $fO_2$: QFM, QFM-2, and IW. Crystallization sequences, modal abundances, and compositional ranges of minerals predicted by each model at each oxidation state were examined for systematic changes with changing $fO_2$.

**Results:** Table 1 summarizes the best-fit model for each composition and highlights the anomalies produced by the other models that suggest they may not be appropriate for such compositions and/or $fO_2$.

**1) Nakhla:** MELTS best reproduced the crystallization sequence for Nakhla at QFM. Liquidus temperatures were approximately the same for plagioclase and pyroxene, but for olivine, it decreased from QFM to QFM-2, then increased at IW. Plagioclase abundances did not vary, but olivine doubled from QFM to QFM-2, then increased only slightly at IW. Spinel decreased from QFM to IW. Augite was the only pyroxene at QFM and QFM-2, and both augite and pigeonite were present at IW. Total pyroxene abundance decreased at QFM-2 then increased at IW. Olivine, plagioclase, and augite compositions were constant from QFM to IW.

Liquidus temperatures using MAGPOX increased for all minerals from QFM to IW, except no plagioclase crystallized at QFM. Modal percentages of augite and spinel decreased from QFM to IW, olivine increased, and plagioclase remained the same from QFM-2 to IW. No significant compositional variation was observed from QFM to IW.

Using COMAGMAT, liquidus temperatures for olivine increased from QFM to IW, decreased for spinel, and varied for augite. Spinel and plagioclase decreased in abundance from QFM to IW. Olivine did not crystallize at QFM, but increased in abundance from QFM-2 to IW. Augite abundances were the same at QFM and IW, but higher at QFM-2. Mineral compositions were comparable for all $fO_2$s.

**2) LEW 86010:** Using the composition for LEW 86010, MELTS was the only model to predict the correct crystallization sequence at all three $fO_2$s. Liquidus temperatures for all minerals decreased from QFM to IW except for olivine, which increased. Abundances of plagioclase decreased from QFM to IW, pyroxene increased slightly, and olivine increased significantly from QFM to QFM-2, but remained the same from QFM-2 to IW. Spinel decreased from QFM to QFM-2, but remained the same at IW. The compositions of plagioclase and pyroxene were virtually indistinguishable at every $fO_2$. Olivine compositions were homogeneous at QFM and the range of Fo contents was greater at IW than QFM-2.

MAGPOX crystallized olivine before plagioclase or augite at every $fO_2$, and liquidus temperatures increased from QFM to IW for nearly all minerals. Modal abundances of minerals were about the same at QFM and QFM-2. From QFM-2 to IW olivine and plagioclase increased and pyroxene and spinel decreased significantly. Plagioclase and pyroxene compositions were consistent from QFM to IW, and olivine compositions decreased only slightly.

COMAGMAT did not predict olivine at any $fO_2$. Augite, plagioclase, and minor spinel crystallized at QFM, augite and spinel crystallized at QFM-2 and augite and trace plagioclase crystallized at IW. Augite compositions and abundances were consistent. Spinel abundances decreased from QFM to QFM-2.

**3) Apollo 15 basalt 15555**: MAGPOX predicted the correct crystallization sequence for 15555 at every $fO_2$. Liquidus temperatures for most minerals increased slightly from QFM to QFM-2, but were unchanged from QFM-2 to IW. Olivine more than doubled in abundance from QFM to QFM-2, but increased only slightly from QFM-2 to IW. Pigeonite and spinel abundance decreased slightly from QFM to IW, and

augite remained the same. Plagioclase abundance decreased slightly from QFM to QFM-2, then remained the same from QFM-2 to IW.

Using MELTS, liquidus temperatures for olivine increased by nearly 200°C from QFM to QFM-2, but remained the same from QFM-2 to IW. Pigeonite, augite, and plagioclase temperatures varied slightly, but within an error of ±10°C. Compositions of most minerals were consistent from QFM to IW except olivine: forsterite contents increased from QFM to QFM-2, but remained the same from QFM-2 to IW. Modal abundances of augite and plagioclase were the same from QFM to IW. Pigeonite and spinel abundances decreased slightly from QFM to IW, and olivine increased slightly from QFM to QFM-2, but were unchanged from QFM-2 to IW.

COMAGMAT showed considerable variation in the type of pyroxene predicted for 15555. Although augite crystallized with roughly the same composition at every $fO_2$, orthopyroxene crystallized at QFM, pigeonite crystallized at QFM-2, and no low-Ca pyroxene crystallized at IW. These differences make it difficult to assess variations in modal abundances of pyroxenes. Olivine crystallized in roughly the same abundance and composition at QFM-2 and IW, but did not crystallize at QFM. Plagioclase crystallized at the same slightly lower temperature at QFM-2 and IW than at QFM and in the same modal abundance and composition at all three $fO_2$s. Spinel decreased in abundance from QFM to IW.

**Conclusions:** Generally, all three models predict comparable mineral compositions, and they do not vary significantly with $fO_2$. Therefore, it is usually the crystallization sequence or modal abundances that determine which model is the best match (Table 1). MELTS and MAGPOX each predict nearly the same crystallization sequence at different $fO_2$s. Because MAGPOX is calibrated for rock types with olivine on the liquidus, olivine will always be the first phase to crystallize. Therefore, the output file must be interpreted correctly for rocks in which a different phase first appears on the liquidus (ex. augite in Nakhla and plagioclase in LEW 86010). As expected, the ratio of olivine/pyroxene abundances increases with decreasing $fO_2$ using MAGPOX. Olivine/pyroxene ratios using MELTS and COMAGMAT, however, are inconsistent. Spinel abundances typically decrease with lower $fO_2$ using all three models, as expected.

As discussed in Part I of this study, igneous crystallization models should not be used with the assumption that one is appropriate for all compositions or magmatic $fO_2$s. Although the internet version of COMAGMAT was used in this study, several versions are available in disk format that have been modified for specific compositions in order to obtain a better fit. Similar modifications can be made to MAGPOX, and presumably to MELTS. Therefore, it is important that the user and the reader understand which version of a particular model was used and for what compositional range it was calibrated or modified.

**References:** [1] Ghiorso M. S., and Sack R. O. (1995) *Contrib. Mineral Petrol., 119,* 197-212. [2] Longhi J. (1991) *Amer. Mineral., 76,* 785-800. [3] Ariskin A. A.. et al. (1993) *Computers & Geosciences, 19,* 1155-1170. [4] Stockstill K. R. (2003) *MAPS,* submitted. [5] McKay G. et al. (1988) *LPSC XIX*, 762-763. [6] Janghorbani M. et al. (1973) *GCA, 2,* 1115-1126.

**Table 1.** Summary of best-fit crystallization models and oxidation states for Nakhla, LEW 86010, and Apollo 15 basalt 15555 (xln seq=crystallization sequence; ol=olivine; pl=plagioclase).

| $fO_2$ | Nakhla (magmatic $fO_2$: QFM-0.5) | | | LEW 86010 (magmatic $fO_2$: IW+1) | | | Apollo 15 555 (magmatic $fO_2$: IW) | | |
|---|---|---|---|---|---|---|---|---|---|
| QFM | **MELTS** | COMAGMAT | MAGPOX | MELTS | COMAGMAT | MAGPOX | MELTS | COMAGMAT | MAGPOX |
| | **best fit** | no ol | wrong xln seq | pl high/ol low | wrong xln seq | wrong xln seq | wrong xln seq | no ol | modal ol low |
| QFM-2 | MELTS | COMAGMAT | MAGPOX | **MELTS** | COMAGMAT | MAGPOX | MELTS | COMAGMAT | **MAGPOX** |
| | wrong xln seq | wrong xln seq | wrong xln seq | **good fit** | wrong xln seq | wrong xln seq | wrong xln seq | wrong xln seq | **good fit** |
| IW | MELTS | COMAGMAT | MAGPOX | **MELTS** | COMAGMAT | MAGPOX | MELTS | COMAGMAT | **MAGPOX** |
| | wrong xln seq | wrong xln seq | wrong xln seq | **good fit** | wrong xln seq | wrong xln seq | wrong xln seq | wrong xln seq | **good fit** |