The Interpretation on Pseudosection calculations using Perple_X Software: A case study of high-grade gneiss in Mogok-Metamorphic Belt

Wai Yan Lai Aung[1] and Thet Tin Nyunt[2]

Abstract

This study represents how do well interpretation on a computer program for *P-T* history of Metamorphic Rocks using Pseudosection approach. Pseudosections are generated on some chemical data and EPMA data taken from the high-grade gneiss in Mogok Metamorphic Belt. The resulted combined data obtains the thermodynamic modeling of metamorphic rocks. Pseudosections are calculated with Perple_X for understanding the evolutionary histories of metamorphic rocks are discussed.

Keywords: pseudosection, Perple_X, computer program, *P-T* history, chemical data, EPMA

Introduction

A bulk composition determined via X-ray fluorescence (XRF) technique is very important and useful in igneous petrology. In metamorphic petrology, this technique is rarely used in Myanmar. The main purpose of the research is how to prepare pseudosection calculations produced by simple experiment on natural rocks: an example from high-grade gneiss of Mogok.

A **pseudosection**, also called an ***equilibrium phase diagram***, is a type of phase diagram that shows the fields of stability of different equilibrium mineral assemblages for a single bulk-rock composition. **Perple_X** is a thermodynamic calculation package suitable for rapidly creating phase diagrams of all types, creating (phase diagrams that include only those reactions experienced by a particular bulk composition). It allows easy estimation of rock and mineral properties as a function of conditions (pressure, temperature, composition).

Obtaining pseudosection modelling by using Perple_X software, there will be basic needs of two main equiptments; X-ray fluorescence (XRF) spectrometer and electron probe microanalyzer.

Methods and Results

Thermodynamic modelling in metamorphic rocks

Thermodynamic functions are associated with Gibbs Free Energy and produce phase diagrams by using software of Holland & Powell, 1991, 1998 (CORK). Thermodynamic modelling of phase equilibria is a powerful technique for estimating pressure and temperature *(P-T)* conditions, for a specific rock composition. However, quantitative application of these techniques requires estimation of the effective bulk composition (Stüwe, 1997) and determination of a chemical system necessary to describe the mineralogical changes accurately in a given *P-T* space. The selection of the chemical system is very important because components that are not considered in modelling may affect phase stability in nature. The minor components influence stability fields, and the variance of assemblages. For example, introduction of Mn into the CaO-FeO-MgO-Al_2O_3-SiO_2-H_2O (CFMASH) system stabilizes garnet at lower pressures and temperatures (e.g., Thompson, 1957; Albee, 1965;

[1] Demonstrator, Department of Geology, University of Yangon,
[2] Deputy Director General, Department of Geological Survey and Mineral Exploration

Spear & Cheney, 1989; Mahar et. al., 1997; Tinkham et. al., 2001). Minor components that contribute to a crystallization of a certain mineral influence the proportions and the chemical composition of other phases in the system. For instance, B stabilizes tourmaline and affects the Na_2O-CaO-K_2O-FeO-MgO-Al_2O_3-SiO_2-H_2O (NCKFMASH) system by reducing the amount of Si, Al, Fe, Mg, Ca and Na available for other minerals. Based on comparison between predictions of thermodynamic modelling in the MnO-Na_2O-CaO-K_2O-FeO-MgO-Al_2O_3-SiO_2-H_2O (MnNCKFMASH) system with predictions in the KFMASH system (Tinkham et. al., 2001) concluded that the nine-component system MnNCKFMASH is the minimum that should be considered for modelling normal garnet-bearing pelitic rock compositions (low-Al and high-Al pelites; Spear, 1993) if retrieval of garnet composition is required. Therefore, most of the pseudosections constructed herein are based on the MnNCKFMASH system. In addition, ten-component pseudosections (MnNCKFMASHT) are provided in order to demonstrate the effects of Ti on peak metamorphic phase equilibria.

Analytical procedures and abbreviations

Before the calculation

To use phase petrology (especially "pseudosections) effectively we need to: Take appropriate samples, Understand the geological context of those samples, Field observations, Undertake chemical analysis of those samples, Whole-rock analyses and Undertake a petrographic study of those samples – thin sections and microprobe analysis. Whole-rock major-element analyses were carried out on the Wave-length Dispersive X-ray Fluorescence Spectrometer (WD-XRF, Axios, PANanalytical), equipped with 5 diffraction crystals at Swiss Federal Institute of Technology (ETH) in Zurich, Switzerland (Fig. 1, A). Minerals were analyzed using the Electron Probe Micro Analyser (EPMA) Jeol, JXA 8200, equipped with SE- and a BSE-detector, 5 WDS crystal spectrometer and an EDS-analyser at Swiss Federal Institute of Technology (ETH) in Zurich, Switzerland. Operation conditions were: 15.0 kV applied accelerating voltage, 100 µm beam size and 10 or 20 nA depending on the stability of the analyzed minerals under the electron beam (Fig. 1, B).

Figure (1) A. Wavelength Dispersive X-ray Fluorescence Spectrometer (WDXRF)

Figure (1) B. Electron Probe Micro Analyser (EPMA)

Authors would like to sillimanite-garnet-biotite gneiss in Mogok Metamorphic Belt is given as an example of sample preparation process for electron microprobe analyses (Fig. 2).

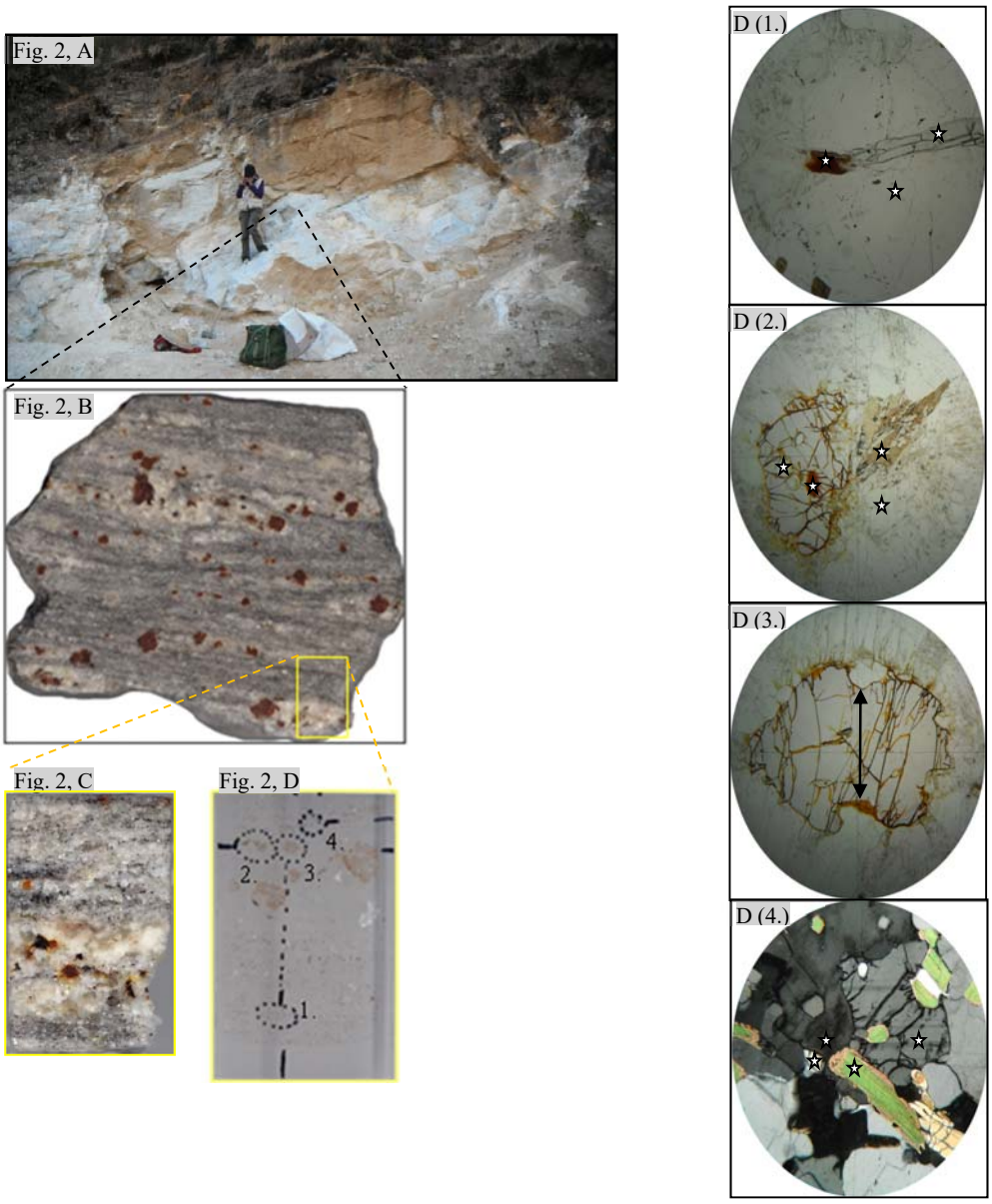

Figure (2). Procedures of electron microprobe analysis process
A) Outcrop nature of sample 1B at the peak of Mount Loi-Sau,
B) Collected hand specimen,
C) Selective chip for thin section,
D) Selected points for EPMA on carbon coated 30 μm thin section,
D,1.) Matrix (Sillimanite, Biotite & Plagioclase),
D,2.) Matrix (Biotite & K-feldspar), and inclusion (Biotite & Quartz),
D,3.) Garnet profile,
D,4.) Matrix (Biotite, K-feldspar, Plagioclase and Quartz).

Modelling instructions

The calculation structure is ***build*** (to define the calculation), ***vertex*** (to run the file made by build), ***pssect*** (to make a PostScript file from the ***vertex*** output). The PS file can be

opened in Ghostview, Adobe Acrobat, Reader or illustrator or the Corel programs). ***Werami*** tells us how the compositions and modal proportions of co-existing phases vary as a function of bulk-rock composition. Calculate the XMg (MgO/(MgO+FeO)) of garnet and modal proportions of melt. Use ***Matlab*** or ***PyWerami*** for plotting the isopleths. The basic approach to creating a diagram in Perplex involves the following sequence of steps:

Abbreviations

The mineral abbreviations (Kretz, 1983) used are Mu = muscovite, Bt = biotite, Qtz = quartz, Grt = garnet, Sil = sillimanite, Pl = plagioclase, Kfs = sanidine, Ilm = ilmenite, Liq = Melt; Alm = Fe/ (Ca + Fe + Mg + Mn), Prp = Mg/ (Ca + Fe + Mg + Mn), Grs = Ca/ (Ca + Fe + Mg + Mn), Sps = Mn/ (Ca + Fe + Mg + Mn), XFe = Fe/ (Fe + Mg), An = Ca/ (Ca + Na + K), Ab = Na/ (Ca + Na + K), Or = K/ (Ca + Na + K).

Calculation methods

To constrain the pressure-temperature (*P-T*) conditions of the study area, phase diagram sections were computed from the bulk-rock composition, the mineral chemistry and the amounts of the constituent phases.

For this section, the model chemical system MnNCKFMASH was used with the bulk-rock composition obtained from XRF analysis. In example sample, MnO was included in the modelling due to its influence on the stability of garnet at low temperatures (Spear, 1993; Tinkham et. al., 2001) although the Mn content of this rock is low (0.1 wt %). TiO_2 was not considered due to its detrimental effect on model proportions of phases at the high-temperature conditions. The amount of H_2O component involved in the calculation for the bulk-rock composition was assumed as the loss of ignition of XRF analysis and thus represents the water content available for equilibration of the observed mineral assemblage.

For inferring the *P-T* conditions of high-grade metamorphic rock, which are sillimanite-garnet-biotite gneisses, the MnNCKFMASH chemical system was used. All the calculations were done by the Gibbs energy minimizing (Connolly, 2009) with the thermodynamic database of Holland and Powell (1998, as revised in 2003). Mixing properties of phases used for the calculation were taken from White et. al (2007) for the solution model of melt, garnet from Holland and Powell (2001), biotite from Tajčmanová et. al. (2009), plagioclase from Newton et. al. (1980), K-feldspar from Thompson and Hovis (1979) and spinel from Nichols et. al. (1992). Procedures of calculation methods to produce *P-T* pseudosection diagrams by using Perple_X computer program (Connolly, 2009) are shown in (Fig. 4).

Results of example sample

Regarding the mineral chemistry, the high-grade metamorphic mineral assemblages in the granulite facies can be treated in the MnNCKFMASH system with quartz in excess. The pseudosection is based on the following molar bulk-rock composition: MnO = 0.37, Na_2O = 0.66, CaO = 0.25, K_2O = 3.38, FeO = 5.83, MgO = 5.87, Al_2O_3 = 9.76, SiO_2 = 68.85, H_2O = 4.29. This composition does not have stability field for spinel (Fig. 5, A) that demonstrates that the whole rock composition is inappropriate for thermobarometric analysis of the high temperature low-pressure assemblages.

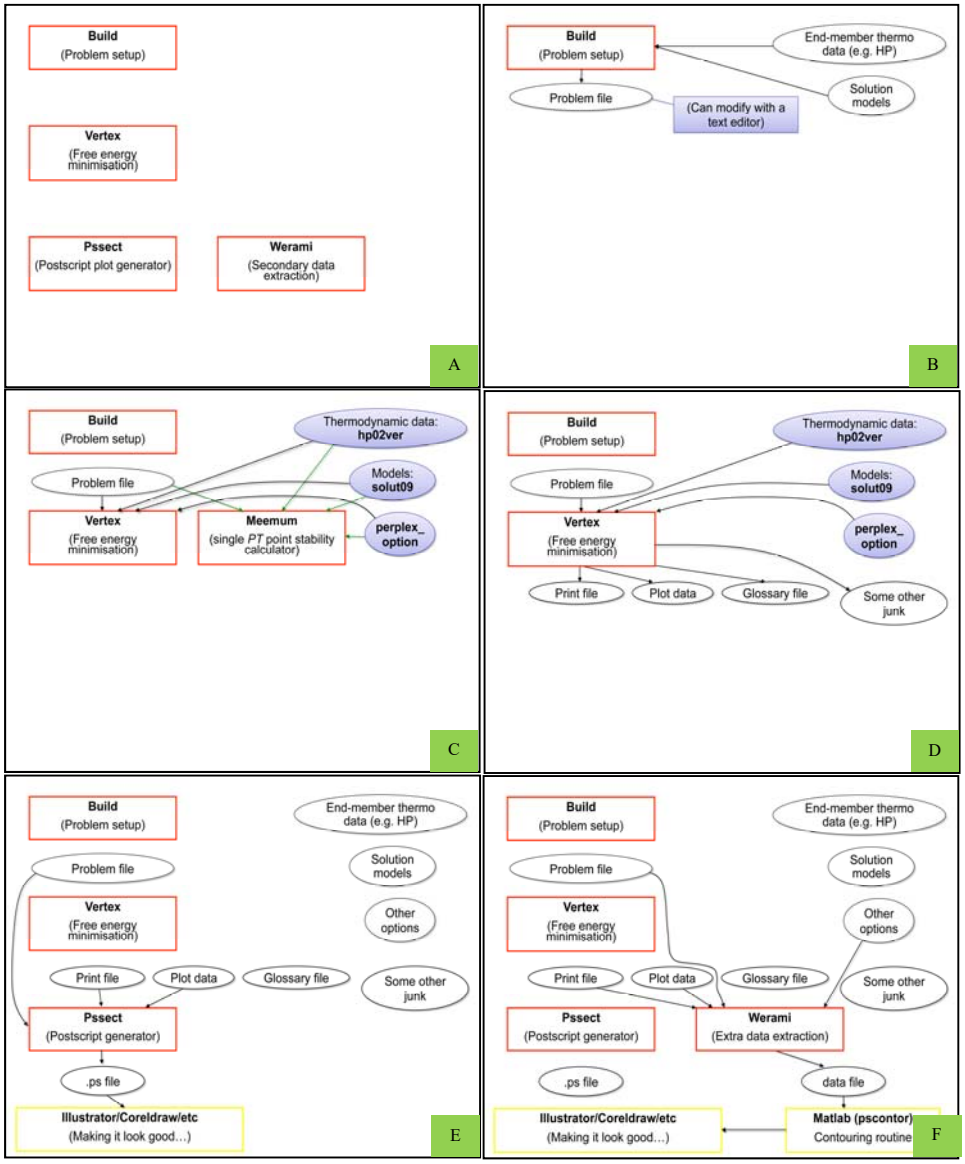

Figure (4) (A - F). Procedures of calculation methods to produce pseudosections by using Perple_X (*Source: ETH web link*).

The calculated pseudosection is simple in geometry, but provides several important constraints about high temperature conditions of the granulite facies. (Fig. 5, A) shows that the granulite facies (e.g. muscovite-free) assemblage can only be present at high temperature conditions, when muscovite is removed from the rock by dehydration melting. The resulting mineral assemblage is biotite-liquid-feldspar-garnet-sillimanite-quartz. In several samples, the crystallization of spinel in domains rimming metastable garnet crystals has been observed. Spinel corresponds to spinel-hercynite solid solution and spinel-bearing mineral assemblages typical of low pressure/ high temperature metamorphism. Isopleths of almandine component in garnet ($X_{Mg0.42\rightarrow0.44}$) with anorthite content in plagioclase (0.01%) and biotite component ($X_{Mg0.59\rightarrow0.60}$) are the only clues to metamorphic conditions at this high temperature metamorphic conditions recorded by the sample, which corresponds to 6.5-9.3 kb at 740-810 ºC (Fig. 5, B).

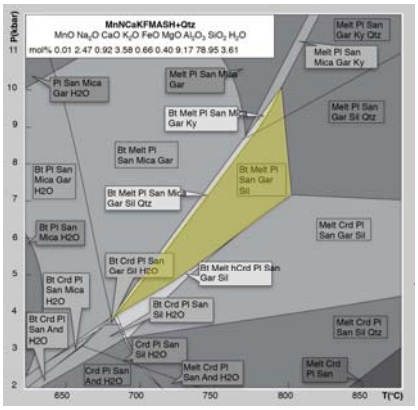

Figure (5A). *P-T* pseudosection for high grade in sillimanite-garnet-biotite gneiss (Wai Yan Lai Aung, 2016)

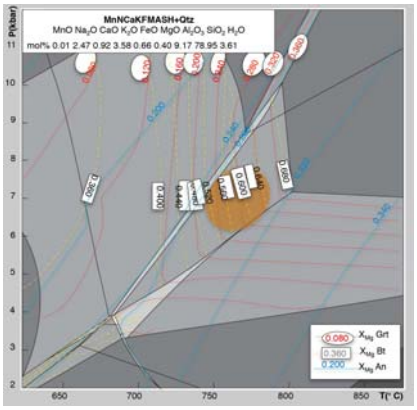

Figure (5B). Isopleths of modal proportions of garnet, biotite and anorthite (Wai Yan Lai Aung, 2016)

Discussions

The influence of bulk composition estimates on P-T pseudosections

The choice of inappropriate bulk composition may critically influence the pseudosection geometry and the position of isopleths in the stability fields of multi-variant mineral assemblages (Stüwe, 1997). In this case, the effective bulk composition covering the mineral assemblage was derived from the regions in thin sections centered on one of the Fe-Mg minerals (garnet in the case of the high pressure sample and sillimanite in the case of high temperature sample) and covering the mineral assemblages. With no local reaction textures present in the studied samples, the only possible error in the effective bulk composition determination can occur due to the inappropriate amount of matrix involved in the estimate. The variation in the stable mineralogy and/ or in the position of isopleths used for the *P-T* estimates can be monitored by adjusting the estimated volume percentage of model mineralogy, regarding high temperature dependence of isopleths in *P-T* pseudosections.

Estimating P-T conditions by phase equilibria modelling

To get the P-T stability field for the study area, firstly need to find the mineral assemblages of analyzed samples on the pseudosection geometry calculated from XRF data. Secondly, X_{Mg} ratio of isopleths such as garnet, biotite, and anorthite percentage of plagioclase, normalized from microprobe data should also be noted. Then, plot a field of overlapping stabilized area with the mineral assemblages and the position of the intersection of the isopleths.

Conclusions

Nowadays, pseudosection modelling is rapidly becoming an essential part of a petrologist's toolkit and often forms a basis of interpreting the tectonothermal evolution of a metamorphic rock sample, outcrop, or geological region. To getting the precise and accurate calculation and interpretation, we do not have to neglect the precautions before calculation such as field study, desk study and lab study. The last but not least is that the interpretation is the result of combined data generated from Perple_X software on both XRF (bulk rock composition) and EPMA (mineral chemistry).

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