On coupling of viscous relaxation and chemical diffusion under grain scale pressure variation

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On coupling of viscous relaxation and chemical diffusion under grain scale pressure variation
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Compositional zoning in metamorphic minerals have been generally recognized as an important geological feature to decipher the metamorphic history. The observed chemical zoning of, e.g. garnet, is commonly interpreted as disequilibrium between the fractionated inner core and the surrounding matrix. Such disequilibrium is caused by sluggish chemical diffusion and reaction rate controlled mainly by temperature under a given amount of time. In principal, at high temperature, where the diffusion coefficient are higher, such a chemical zoning should be erased. Paradoxically, chemically zoned minerals were also observed in high grade rocks (T>800°C) where the duration of metamorphic processes was independently dated to take several Ma. This implies that temperature may not be the only factor, and grain scale pressure variation was proposed to be a complementary factor that may significantly contribute to the formation and preservation of chemical zoning in high temperature metamorphic minerals [Tajcmanová 2014, 2015].

However, the common petrology view is that the viscous relaxation in rocks is fast and therefore homogeneous pressure is still commonly assumed in the quantification of metamorphic processes. Here, classical irreversible thermodynamics is used to model viscous relaxation coupled with chemical diffusion. The numerical approach is applied to the chemically zoned plagioclase rim described by [Tajcmanová 2014]. We document the effect of density differences between plagioclase end members during the chemical diffusion on pressure distribution across the evolving microstructure. The diffusion process operating during the plagioclase rim formation can thus lead to a development of a pressure gradient. Such a pressure gradient if maintained during ongoing viscous relaxation can lead to the preservation of the observed chemical zonation in minerals.

Numerical approach

The model length (Lx), adiabatic bulk modulus (K), and diffusion coefficient (D) are chosen as scales to non-dimensionalize the governing equations. Substitution of the scaled parameters into the equation enables us to write dimensionless Deborah number and dimensionless time respectively as De = \( \frac{D\eta}{Lx^2K} \) and \( t' = \frac{tD}{Lx^2} \). All the dimensionless parameters such as pressure are resumed back to dimensional value at the end of the approach. In contrast to commonly used Deborah number of Maxwell relaxation time divided by thermal relaxation time, this Deborah number is an expression of Maxwell relaxation time (\( \frac{\eta K}{Lx^2} \)) divided by the characteristic diffusion time (\( \frac{Lx^2}{D} \)). This parameter is designed to characterize the relative influence from viscous relaxation and diffusive process. Small De implies relatively fast viscous relaxation (low \( \eta \)) and slow diffusion (low D). This represents the conventional petrological point of view that rocks cannot preserve pressure gradient due to fast viscous relaxation. Large De indicates the opposite situation of slow viscous relaxation and fast diffusion as proposed by [Tajcmanová 2014, 2015]. We can systematically investigate the system by varying De, up to a certain \( t' \) to characterize the behavior of the system under initial pressure gradient.

Model setup and results

We applied our numerical approach to a zoned plagioclase rim described by [Tajcmanová 2014]. The initial model setup is illustrated in Fig. 1 for pressure, and anorthite concentration. The temperature is fixed at 800°C, thus thermal diffusivity is not relevant to our model. The model runs at dimensionless De = \( \frac{D\eta}{Lx^2K} = 2.3 \) and \( t' = \frac{tD}{Lx^2} = 0.85 \) in Fig.1, and is also printed as yellow stars in Fig. 2. The initial gradient of chemical potential difference indicates that diffusion will
immediately occur, thus leading to a perturbation of pressure coupled by equation of state. Pressure is eventually preserved due to the large Deborah number, thus form chemical zonation at high temperature.

![Graph of Dimensionless Pressure vs Dimensionless x](image1)

![Graph of Concentration vs Dimensionless x](image2)

**Fig. 1** The initial setup of pressure is flattened and the initial concentration is given by a simple Gaussian function. Chemical potential is calculated by thermodynamic database of [Holland and Powell 1998] using Perple_X [Connolly 2009]. Although the model is run with dimensionless setting, the plotted variables here are converted back to dimensional.

In Fig. 2, it can be clearly observed that pressure and concentration variation can be preserved at high $De$ (top half of the images), which indicates slow viscous relaxation and fast diffusion. In case of low $De$ (bottom half of the images), fast viscous relaxation permits no pressure variation to be created and preserved. As for Fickian diffusion case, $De$ is not influential as diffusion is purely driven by concentration gradient, thus it is free from any pressure gradient influence. Any results of dimensional variables can be represented within the dimensionless diagram in Fig. 2.

**Fig. 2** Preserved pressure, concentration and Fickian concentration of anorthite variation (maximal minus minimal) plotted as functions of dimensionless time and the Deborah number. The yellow star represents the parameters of Fig. 1.

**Conclusion and Outlook**

We simulate viscous pressure relaxation coupled with diffusion to investigate the formation and preservation of the zoned binary plagioclase. It is documented that the chemical diffusion during the growth of the plagioclase rim can generate pressure gradient and the generated pressure gradient can then be preserved over Ma timescale to concomitantly hold the chemical zonation. Future work will involve ternary, and quaternary garnet model, coupled with reactive fluid rock interaction to fully investigate the formation and preservation of zonation considering other matrix phases.
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Reference