

Calculation of the Model of Coesite Inclusions and Analysis of Their Retrometamorphic Paths

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Abstract The process and path of retrometamorphism of coesite have great significance to our understanding of the P - T tracks of the exhumation of ultrahigh-pressure metamorphic rocks. Most of the coesites in the eclogite from Shima, Anhui Province, the Dabie Mountains, China, are found degraded to quartz partly or wholly, with ruptures occurring in the shells, outside which include the coesite and quartz. According to the microscopic observation, the sample of coesite inclusion is composed of garnet, quartz and coesite, based on which we have built a three-shelled composite sphere model to compute the transition of coesite. Based on the crystal growth formulas and pressure conditions of the ruptures in the garnet, we have calculated the radius of the quartz sphere, which depends on temperature, and eventually drawn the different retrometamorphic paths for different retrometamorphism rates.

Key words: ultrahigh-pressure metamorphic rocks, coesite, model calculation, retrometamorphic path, Dabie Mountains

1 Introduction

Up to now, geologists have found many coesite inclusions in rocks located in worldwide ultra-high pressure (UHP) metamorphic terrains, most of which are degraded to polycrystal quartz partly or wholly. They are included in garnet, zircon or omphacite hosts. As an inclusion, coesite occurs in three forms: Firstly, it is totally transformed into quartz with radial ruptures of the garnet host; secondly, it is partly transformed into quartz along the rims of residual coesite also with radial ruptures of the garnet host; thirdly, some well-preserved coesite crystals are found in zircon or garnet inclusions without any rupture.

Belonging to the monoclinic form, coesite has a pseudo-hexagonal crystal scale (SiO_2 , $a=0.717$ nm, $b=1.238$ nm, $c=0.717$ nm, $\beta=120^\circ$, $C2/c$, Zoltai et al., 1959). However, neither three- or six-rings nor spirals exist in the crystal structure (Meng and Han, 2000; Langenhorst and Poirier, 2002).

Most researchers believe that the retrogression of coesite is attributed to the changes of pressure and temperature. Having experienced the unstable period during the exhumation, coesite is finally transformed into quartz. Recently it is reported that fluid may be the factor which controls the varying degree of coesite-quartz transition (Ye et al., 2001). However, no water has been found in natural coesite with the FITR (Fourier-transform infrared) (Monsenfelder, 2000) and the experiments suggest that coesite is unlikely to be preserved in geological times in the quartz stability field when the temperature exceeded

375–400°C with fluid activity (Monsenfelder and Bohlen, 1997). Under the action of fluid coesite will transform wholly into quartz in hours or days. Therefore, fluid may enter into the coesite only in the later period of retrogression. The retrogression of coesite is considered to be controlled by its nucleation and growth. Coesite becomes metastable during the descension of temperature and pressure. Quartz nucleates in coesite and grows into a retrometamorphic quartz inclusion.

2 Model of Elastic Sphere Built for Garnet-Quartz-Coesite Inclusions

The sample comes from coesite-bearing eclogite in Shima, Anhui Province, Dabie Mountains, China. As shown in Fig. 1 the coesite inclusion is composed of coesite, retrometamorphic quartz and garnet host. The quartz, which is degraded from coesite, nucleates and grows around the relic coesite at equal thickness and radial ruptures occurs evenly in the outer host. It can be concluded that the conditions of nucleation of quartz are the same on the surface of coesite and the radial growths around the surface are nearly synchronous.

In the present paper the coesite-garnet inclusion is analyzed by using the model of a composite sphere consisting of three shells (Fig. 2). Based on an observation by the microscope, the initial radii of coesite shell, quartz shell and garnet-host shell are respectively taken as: $R_c(0) = 0.5 \times 10^{-4}$ m, $R_q(0) = 0.5 \times 10^{-4}$ m and $R_g(0) = 10^{-2}$ m.

The pressure inside the garnet shell will increase with the

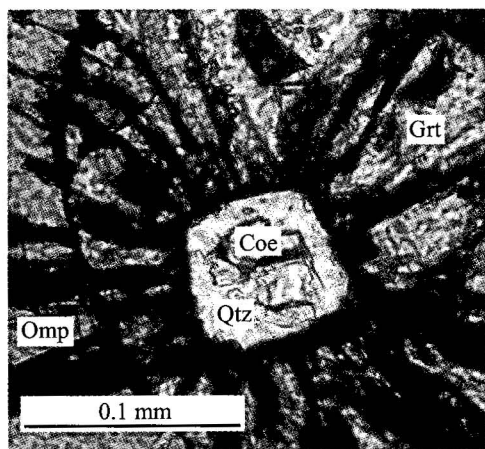


Fig. 1. The photomicrograph of a coesite inclusion from Shima, Anhui Province, China.

coesite-quartz transition as the volume expands, while the initial overpressure in garnet is much lower than 0.05 GPa (Ye et al., 2001). The model is computed for the temperature range from 1000 K to 600 K, and the initial pressure can be ignored (lower than 0.05 GPa).

3 The Occurrence of Rupture in the Garnet Host

First of all, we have to consider the effect of decreasing temperature and pressure on the radii of the shells, because the bulk variety caused by temperature and pressure may lead to the rupture of the garnet host. During the exhumation of ultra-high pressure metamorphic rocks including the garnet-coesite inclusions, the temperature decreases from 1200 K to 298 K and the pressure decreases from 2.8–3.0 GPa to 0.1 MPa. When the pressure decreases, the garnet shell and coesite shell will have a bulk expansion in their elastic range, but it gives no obvious overpressure in the inclusion. The decrease in temperature leads to a bulk compression in the garnet shell. The decrease of the radius is calculated as $\Delta S = \beta \cdot \Delta T \cdot R_C(0)$ (β is the rate of linear expansion of garnet taken as $5.31 \times 10^{-6}/\text{K}$) (Xiao and Wang, 1989). When the temperature varies from 1300 K to 298 K, ΔS is about $2.389 \times 10^{-7} \text{ m}$ and the decrease of bulk is about $7.501 \times 10^{-15} \text{ m}^3$. It can only produce an overpressure of less than 0.1 GPa. To cause rupture in the garnet shell the overpressure should be at least 2.4 GPa. Therefore, the only reason for producing rupture in the host is the overpressure between the garnet shell and the quartz shell caused by volume expansion during the coesite-quartz transition (Gillet et al., 1984).

When the overpressure caused by transformation reaches $\Delta P = 2.4 \text{ GPa}$, the garnet shell cannot endure and rupture occurs. If the molar volume ratio of quartz (α) and

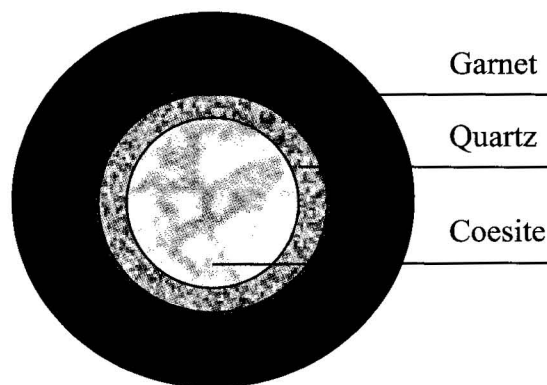


Fig. 2. The model of a compound sphere of coesite-quartz-garnet inclusion.

coesite is taken as 22.68/20.75 (≈ 1.093) (Cheng et al., 1995), an equation about the transformation rate ε can be written as:

$$(1.093 - 1) \varepsilon = \Delta P / U$$

where U , the bulk modulus of quartz, is taken as 37.8 GPa (Nishiyama, 1998). When rupture occurs, the radius increment of the quartz shell is calculated as:

$$\Delta R_Q = \sqrt[3]{1 + 0.093 \varepsilon R_0} - \sqrt[3]{1 - \varepsilon R_0} \approx 0.169 \times 10^{-4} \text{ m}$$

$$(R_0 = 0.5 \times 10^{-4} \text{ m}).$$

4 Growth of the Quartz Shell

During the process of coesite-quartz transition, quartz nucleates at the dislocation or interstice in the coesite and grows into polycrystal quartz. Quartz nucleates easily on the surface of coesite because of the lower energy demanded for nucleation on the surface than in the interior. Therefore, the nucleation starts from the surface of coesite and grows towards the core of the coesite shell with the consumption of coesite. As is often pointed out, nucleation in solid only needs several seconds, especially at a high temperature. Compared with the retrogression history of millions of years, the nucleation process can be thought instantaneous (Xu, 1988; Monsenfelder and Bohlen, 1997). The transformation of coesite is thought to be a growth process of quartz on the surface of the coesite shell which is controlled by short-distance diffusion of atoms. Assuming that the process begins at temperature T_0 (K), the radius increment of the quartz shell can be described by (Monsenfelder and Bohlen, 1997):

$$\Delta R_Q = \int_{t(T_0)}^{t(600)} \{ K_0 T [1 - \exp(-\frac{\Delta G_f}{RT})] \exp(-\frac{Q}{RT}) \} dt \quad (1)$$

where K_0 is a constant (0.185), Q , about 243 KJ/mol, is the activation energy for growth, the constant R is 8.31 J/mol·K, ΔG_r , which is estimated to be 854.872 J, is the free energy of coesite-quartz transformation per mol (Helgeson et al., 1978).

Since K_0 is unknown, Monsenfelder and Bohlen (1997) fitted his experimental data to the equation and got the value for K_0 (0.185). The polycrystalline coesite aggregate has an average fluid content of $294 \pm 111/10^6$ Si for the coesite in this experiment is synthesized from silica glass. These defects in synthesized coesite caused by $-\text{OH}$ or H_2O provide dislocations for nucleation and growth. Compared with natural coesite the ratio of fluid content is about 300 in case of no fluid observed in natural coesites (Monsenfelder and Bohlen, 1997; Monsenfelder, 2000). The discrepancy must be considered when the above equation is used to calculate our natural coesite samples. Thus the equation for the radius increment of the quartz shell is modified as:

$$\Delta R_Q = \frac{1}{n} \int_{r(T_0)}^{r(600)} X dt = \frac{1}{n} \times \sum_{i=1}^N \left\{ K_0 T_{i-1} \Delta t \times \left[1 - \exp\left(\frac{-\Delta G_r}{RT_{i-1}}\right) \right] \exp\left(\frac{-Q}{RT_{i-1}}\right) \right\} \quad (2)$$

where n is the ratio of dislocation density ($n = 300$).

5 Conclusions and Discussion

The temperature variation rate of the UHP metamorphic terrain in the Dabie Mountains ranges from 0.2 K/Ma to 6.5 K/Ma according to the conclusions of You et al. (1996). We take the rate of 5 K/Ma in this paper. If the temperature interval is 5 K, the time increment will be 1 Ma ($\Delta t = 10^6$). We calculated the growth process from 800 K to 600 K and got the radius increment of the quartz shell as more than 1000 μm , which is a meaningless result that only implies that coesite is exhausted. Different initial temperatures such as 740 K, 730 K, 720 K, 715 K and 700 K are fitted to equation (2) to calculate the increasing radius increment of the quartz shell, which is shown in Fig. 3. We have obtained the following results:

(1) When the coesite-quartz transition begins at a initial temperature above 740 K, coesite will transform into quartz without relic during the exhumation.

(2) Only when the initial temperature is above 715 K, will the radius increment of the quartz shell be above 0.169×10^{-4} m, which is the minimum to radial rupture of the garnet host.

(3) If the initial temperature is lower than 715 K, the volume expansion is not sufficient to rupture in the garnet host.

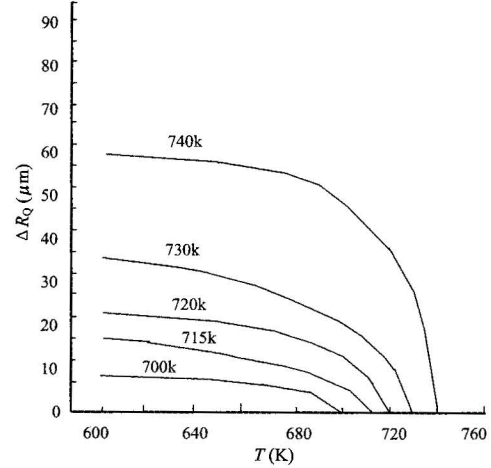


Fig. 3. The radius increments of quartz shells computed at different initial temperatures.

(4) When the temperature is below 650 K, the growth rate will approach zero and the coesite-quartz transition may cease. In this way the coesite will be preserved without transformation.

According to the relationship between the initial temperature and the degree of transformation we have drawn the different P - T paths of coesite-quartz transition during the exhumation (Fig. 4). As showed in the figure, most coesite inclusions experience retrogression path 1 and transform into poly-quartz wholly in the garnet or omphacite host. Some experience path 2 during the exhumation and form degraded quartz around the residual coesite. Others follow path 3 along the equilibrium boundary between the coesite and quartz field and these coesite inclusions can be preserved below 650 K because the rate of diffusion and growth is close to zero. Coesites have been found in UHP metamorphic rocks as inclusions and ascend to ground surface with the exhumation of rocks. Therefore the P - T paths of coesites, which reflect the exhumation paths of the metamorphic rocks, are of great

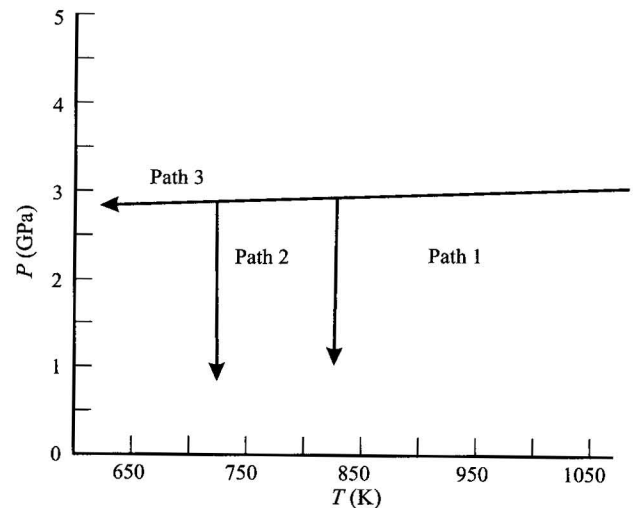


Fig. 4. The retrometamorphic paths of coesite.

significance to the research on the movement of UHP metamorphic rocks.

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