Calculation of the strain, stress and elastic energy for low-high quartz transition up to 1.1GPa

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Considering all the rock-forming minerals in the crust, quartz is probably the most abundant one. The physical and chemical properties of quartz have been extensively investigated. This paper is particularly concerned with the strain, stress and elastic energy in low-high quartz transition at the pressure range of crust.

Procedure of Calculation

As the low-quartz is transformed into high-quartz, the components (e_i) of the strain tensor is: $e_1 = e_2 = a / a_0 - 1$, $e_3 = c / c_0 - 1$, $e_4 = e_5 = e_6 = 0$, where a_0 and c_0 are the cell parameters of low-quartz, and a and c are the cell parameters of high-quartz.

The relationship between an applied stress, σ_i, and the resultant strain, e_k, and the temperature, T, is given by the generalized Hook's low: $\sigma_I = C_{ij}e_k - C_{ij}\alpha_j T$, where C_{ij} are the elastic constants, α_j are thermal expansivities. The elastic energy, G, stored in the crystal is:

$$G = 1/2\sum_{i,k} C_{i,k} e_i e_k$$

The variations of the lattice parameters of low- and high-quartz at high pressure and high temperature can be evaluated with the compressional and thermoelastic properties of low- and high-quartz. Combined the boundary of low-high quartz transition with the results of evaluation, the lattice parameters of low- and high-quartz at their transition pressure and temperature are determined firstly. Then, the strains, stresses and elastic energies for low-high quartz transition were calculated according to Hooke's law with the aid of the elastic constants of high quartz.

Results and Discussion

The results indicate that at the pressure of 0-1.1 GPa, the strains for low-high quartz transition are varied in the range of –0.006-0.005, the stresses in the range of –0.46-0.14 GPa, and the elastic energies in the range of 965-2760 kJ / m^3. At about 0.5 GPa, the strains, stresses and elastic energies achieved their minimum values. Based on the calculation, the effect of the low-high quartz transformation on the wall rock is significant in the crust during the acid magma intrusion.

Reference

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Groundwater Recharge in Late Pleistocene and Holocene at Yucca Mountain, Nevada USA

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The deep unsaturated zone beneath Yucca Mountain is proposed as the site of a geologic repository for high-level nuclear waste in USA. Reliable estimates of recharge at the local scale are important because infiltrating waters provide a potential means for mobilization of radionuclides. The chloride mass balance (CMB) method has been used for estimating groundwater recharge at Yucca Mountain. CMB is economic and effective, provided that the hydrological conditions for its applications are met and the modeling parameters are known. However, modeling parameters such as precipitation and Cl^- deposition rates vary temporally, most notably as a result of the drastic climatic changes from late Pleistocene to Holocene. A common practice in the application of the CMB method is to use present day average precipitation and effective Cl^- deposition rates to calculate recharge rates without regard to the age of the groundwater. This study shows that Cl^- deposition rates, estimated from 36Cl data, were lower in late Pleistocene than Holocene at Yucca Mountain, Nevada, but higher in late Pleistocene than Holocene at Black Mesa, Arizona, another arid environment where hydrological data are abundant.

Temporal variability of atmospheric Cl^- input, as well as annual precipitation, was considered in this study to estimate recharge rates using the CMB method. The resulting average recharge estimates for Black Mesa are 9 mm/yr for Holocene and 35 mm/yr for late Pleistocene. Local recharge rates at Yucca Mountain were estimated from the 36Cl/Cl ratios and Cl^- concentrations in perched waters. The estimated recharge for Yucca Mountain is 5 mm/yr for Holocene and 15 mm/yr for late Pleistocene. Although there is uncertainty in these estimates, greater confidence can be placed in the relative rates of recharge estimated for the late Pleistocene and the Holocene. These estimates agree well with spatially and time-averaged net infiltration estimates for present-day and glacial-transition climates (4.6 mm/yr and 15.6 mm/yr, respectively) obtained from a watershed-scale infiltration model of Yucca Mountain. [This work, performed in part under U.S. Nuclear Regulatory Commission (NRC) contract NRC-02-97-009, does not necessarily reflect views or position of the NRC.]