

Strain energy model for diffusion compensation in mineral

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Diffusion is expressed as $D=D_0\exp(-Q/RT)$, where D_0 is pre-exponential factor, and Q is activation energy. A positive correlation between $\ln D_0$ and Q was observed in many minerals, known as the compensation effect. Thus, there is a critical temperature T_c at which all species have identical diffusion rates, which is useful for understanding closure temperature for diffusion in petrogenetic processes. Although the origin of compensation effect is still unclear, Bejjina and Jaoul¹ proposed a strain energy model to explain the occurrence of the compensation effect during Si diffusion in silicates, and estimated critical temperature T^* as

$$\frac{1}{T^*} = -\left(\alpha_D + \frac{\partial \mu_D}{\mu_D^0 \partial T}\right), \quad (1)$$

where α_D is the local coefficient of bulk thermal expansion, μ_D is the local shear modulus, μ_D^0 is the value of μ_D at $T=0$. Generally, α_D and μ_D are not available. Thus corresponding bulk thermal expansion coefficient α and shear modulus μ was used. We use the average values of $\partial \mu / \partial T$ and α in the temperature and pressure range of study, the calculated critical temperatures T^* of forsterite, zircon, quartz and orthoclase are 1765, 1582, 2196 and 1612 K, respectively. Comparing to their corresponding critical temperatures $T_c = 1656, 1617, 1739,$ and 1623K , there is a significant linear relation between T^* and T_c (see Fig. 1), which shows a reasonable validity of the strain energy model for diffusion compensation in these minerals.

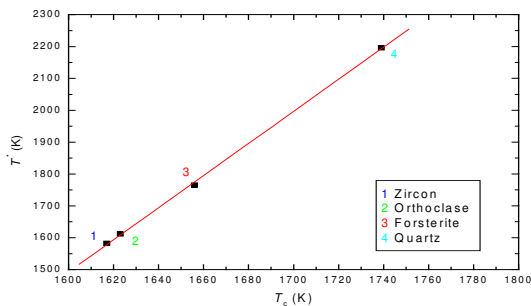


Fig. 1 calculated critical temperatures T^* vs T_c

Acknowledgements:

This work was supported by funds from the Natural Science Foundation of China(No. 40537033, 40374025) and Program for New Century Excellent Talents in University (NCET).

References

- [1] Bejjina F. and Jaoul O. (1997) *EPSL* **153**: 229-238