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A new stress analysis method: Estimation of stress state in a Kawai-type apparatus

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In high-P/T in situ X-ray observation using Kawai-type apparatus, generated pressure is usually determined from the unit cell volume of pressure standard materials, such as cubic crystals of Au, Pt, NaCl and MgO. However, possible deviatoric stress exerting on the standard causes serious error to the calculated pressure. In order to determine the appropriate pressure, it is indispensable to evaluate stress state of the standard material. By analyzing difference among strains of d-spacings, deviatoric stress in the sample can be evaluated from Hooke's law if elastic constants of standard material are known. Here we propose a new simple analysis method to estimate magnitude of deviatoric stress in a Kawai-type apparatus.

The present analysis is a fully numerical approach, and is essentially based on an axial coordinate transformation of the 4th rank tensor of compliance elastic constants, under the assumptions that stress state is axial symmetric and is uniform (Reuss limit). Magnitudes of pressure and deviatoric stress are simultaneously determined from d-spacings of (111) and (200). These d-spacings are invariant with respect to the rotation of crystal grains in the stress field around the axis normal to the diffracted planes; i.e. which are free from preferred orientation. Other hkl reflections, such as (220) and (311), do not keep these special characters. However, in another point of view, analysis of these reflections provides us future possibility of evaluating degree of preferred orientation under non-hydrostatic stress state.

Stress states of the MgO pressure standard in a Kawai-type apparatus equipped with sintered diamond recently adopted by Kubo et al. (2003) were analyzed up to 39 GPa along temperature cycling process from 300 to 1850 K. Our results showed that maximum deviatoric stress at room temperature was 2.2 GPa at the corrected pressure of 35.1 GPa, and that at high temperature was 0.5 GPa at 1740 K and the corrected pressure of 39.3 GPa. The magnitude of the pressure correction was found to be usually comparable with that of deviatoric stress.

Singh (1993) proposed a sort of X-ray stress analysis to estimate deviatoric stress in the sample in an opposed anvil device such as diamond anvil cell. His approach is also an inversion of strains of d-spacings to stress state, but assuming effective elastic constants for each diffraction planes with following two assumptions: (1) non-preferred orientation of crystal grains and (2) Reuss limit or uniform strain (Voigt limit). By comparing the present results with those derived from the method after Singh (1993), it has become clear that the formula for calculating effective elastic constants are accurate only for (200) and (220).

References

Kubo, A. et al., In situ X-ray observation of iron using Kawai-type apparatus equipped with sintered diamond: absence of beta phase up to 44 GPa and 2100 K. Geophys. Res. Lett., in press (2003).

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