Geophysical Research Abstracts, Vol. 8, 00630, 2006
SRef-ID: 1607-7962/gra/EGU06-A-00630

1 Impurity diffusion and microstructure of diamonds deformed at HPHT conditions

A.A. Shiryaev (1), D. J. Frost (2), F. Langenhorst (2)

(1) Institute of crystallography, Leninsky Pr. 59, 119333 Moscow, Russia;, (2) Bayerisches Geoinstitut, Bayreuth, Germany (shiryaev@ns.crys.ras.ru; phone +7495 1355450)

Nitrogen is a principal and the most studied impurity in diamonds; its concentration may reach several thousands at.ppm. It is incorporated into the diamond lattice as single substitutional atoms (so-called C-defect) or as a pair (A-defect) (Shiryaev et al., 2005). Diffusion during annealing leads to formation of more complex defects: the A- and B-defects (4N+V) ("nitrogen aggregation"). The aggregation kinetics was experimentally studied, but considerable discrepancies between values of activation energy of diffusion and other parameters still exist. The degree of the N aggregation is used for estimation of Time-Temperature history of diamond storage in the mantle and thus the N diffusivity has to be better constrained and processes responsible for its acceleration/retardation should be studied. It is known that the absolute majority of natural diamonds are plastically deformed. In this presentation results of experimental investigation of influence of diamond microstructure on nitrogen and hydrogen diffusion are reported. We compare the N aggregation rate in diamonds annealed under quasihydrostatic conditions with annealing in strong strain fields.

Synthetic diamonds (type Ib) were annealed at 1600˚Ñ and 6.5 GPa using a multianvil setup at BGI. Control chips from the samples were annealed in MgO (quasihydrostatics), and other chips were heavily deformed during annealing by using special sample assembly (Cordier and Rubie, 2001) and hard pressure-transmitting medium. The samples were studied using Infra-red (IR) microspectroscopy, X-ray topography, and TEM. Prior to the experiments diamonds were of very high quality and individual dislocations and stacking faults were resolvable in topographs. The annealing or cold compression in MgO does not alter the crystalline lattice quality significantly, but the deformation experiments induce very high stresses.

The microstructure of deformed diamonds strongly depends on the pressure transmitting medium. Annealing in hard silicates (e.g., Ol+Gt) produces mechanical twins, but the dislocation density is low. However, when SiC or diamond powders were used as deforming medium, numerous glide dislocations are produced. Remarkably, the dislocations are heterogeneously distributed and domains of high crystalline quality coexist with heavily deformed regions.

Despite clear microstructural differences, the measurements of the N diffusion rates are less conclusive. Whereas in some cases the aggregation state in heavily deformed diamonds is indeed higher than in non-deformed, in some stones the difference is only marginal and might be explained by slight temperature differences between the experiments. This result indicates that at our PT conditions nitrogen-dislocation interaction is either weak or strongly depends on presence and abundance of vacancies and interstitials as well as their charge state.

Comparison of our experimental results with observations on natural samples suggests that microstructure of diamonds could be an important factor for diffusion in some cases. It is likely, that in zones of plastic deformation the nitrogen diffusion may be faster, whereas numerous stacking faults separating almost perfect crystalline domains inhibit diffusion.

AAS acknowledges support of Alexander von Humboldt foundation. X-ray topographs were acquired at ANKA synchrotron source (Karlsruhe, Germany).