

The kinetics of defect aggregation in diamond. Unlocking the history in natural diamonds.

Many different types of defect have been identified in diamond. Some of them are well-understood but others remain enigmatic, with unknown structures or chemistries and with no established method to relate the magnitude of a spectroscopic observation to the concentration of the associated defect. A complete understanding of defects in diamond is desirable for many reasons, including the effect of different defects on the material properties, as an aid to gemologist in identifying synthetic and treated diamonds and as a tool for the geologist to learn about the deep interior of the Earth.

Some defects in diamond evolve with time from one defect to another. The rate of change depends on the mechanism of the defect reaction and temperature. Nitrogen is of particular importance in diamond, and there has long been interest in the evolution of defects involving nitrogen. However, a complete and quantitative understanding has been hampered by experimental and analytical difficulties. Nitrogen is incorporated into growing diamonds in the form of single substitutional nitrogen. During high temperature annealing these single nitrogens combine to form nitrogen pairs (A-centres) and over much longer timescales A centres combine to form groups of four nitrogen atoms around a vacancy (B centre). The aim of this project is to calibrate experimentally the rate of reaction of the two main defect reactions involving N and to assess the role of other defects that may be involved either as catalysts or as by-products.

There are two key factors in working out the controls on nitrogen aggregation rate. The first is accurate and precise control of temperature and pressure in annealing experiments, the second is quantitative measurement of the concentrations of all the defects involved in both sides of the chemical reaction. The success of the project will depend on technical developments in both areas and the objectives can therefore be broken down as follows.

Objective 1. Development of a new high-pressure and temperature cell for stable annealing of diamonds at temperatures above 2100 °C for extended periods of time. The student will spend several periods of time at the Geophysical Laboratory, Washington D.C., which is known as a world leading lab in high pressure and temperature technologies. The state-of-the-art methods will be imported to Bristol by the student and further development work will take place on the two multi-anvil presses in the experimental petrology laboratory in the School of Earth Sciences.

Objective 2. To refine the quantification of defect concentrations using spectroscopic methods.

Objective 3. To establish an improved kinetic equation for the C to A aggregation process and to study the effect of composition on the rate.

Objective 4. To provide new data on the rate of A to B aggregation

There will be three main applications of the data. The first is in technological applications, where it may be beneficial to manipulate the defects in diamond to optimise a particular property. The second is in gemology where it is vital to be able to distinguish natural diamonds that have been annealed naturally in the Earth's mantle from (i) natural diamonds that have undergone artificial heat treatments and (ii) synthetic diamonds that have processed at high temperatures to change their defect structures. The third application is in geology where the defects present can be used to read the geological history of diamonds and derive key information about the distant past of our planet.

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