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Formation and evolution of nitrogen and hydrogen defects in natural diamonds

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Nitrogen (N) and hydrogen (H) defects in natural diamonds provide fundamental information about diamond growth, diamond-forming fluids and the behavior of volatiles in the deep Earth. The identity of the major N-defects serves as the basis for the *Type Classification* scheme of diamond and determination of the sequence (***C***- to ***A***- to ***B***-centers), and rates by which N-defects evolve (aggregate), allows thermochronometric calculation of the time/temperature history of diamond residence in the mantle. However, the majority of diamonds studied for geologic purposes are highly aggregated (e.g., *Type IaAB*) containing N/H-defects that have evolved during prolonged mantle annealing periods towards their most thermodynamically stable "end-point". Consequently, the mechanisms of N/H incorporation during diamond growth and the sequences of N/H-defect aggregation remain poorly understood.

To address this problem, we filtered >200,000 FTIR spectra (from the *Gemological Institute of America* database) to find spectra from rare *Type Ib* diamonds that reflect N/H-defect aggregation states shortly after diamond formation. This allowed the identity and behavior of newly discovered N-related defects, such as the ***Y***-center, to be constrained. The ***Y***-center is interpreted as a form of single-substitutional N associated with interstitial N_i and C_i that forms as an intermediate product of ***C***-to-***A*** aggregation. Calculation of the ***Y***-center absorptivity allowed development of more precise methods for the calculation of N content and mantle residence temperatures for *Type Ib* diamonds. Moreover, two new H-related defects (NH^0 and N_2H^0) were identified and their structures were determined using novel *ab initio* simulations, including machine-learning molecular dynamics. These H-defects are likely the first to form in diamond, where trapping of interstitial H_i by N-defects acts to modify normal N-aggregation sequences. With progressive annealing, these H-related defects aggregate towards the more stable N_3VH^0 defect implying that once trapped, H cannot re-equilibrate via diffusive loss during mantle residence. Our results define a "starting-point" for the evolution of N/H-defects allowing their behavior to be modelled in future work from the moment of diamond formation through high-temperature mantle residence.

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