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Diffusion of helium in diamond at mantle conditions: new insights from molecular dynamics simulations

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Impurities and mineral/fluid inclusions in natural diamonds can provide valuable insights into the evolution of mantle conditions through geologic time [1]. For instance, the isotopic composition of the early mantle can be inferred by studying helium (He) in diamonds, which may occur in fluid inclusions or as interstitial defects in the diamond lattice. However, a critical aspect to consider when studying He in diamonds is whether or not their isotopic composition is representative of the original diamond-forming fluid. Since most diamonds experience prolonged mantle residence times at high temperature, re-equilibration of He with the surrounding mantle may occur via diffusive loss or gain. Several studies on He diffusion in diamond report contradictory results in activation energies for diffusion (which can vary over an order of magnitude) and in He diffusivities, mainly due to experimental shortcomings including graphitization during high temperature measurements, release of He after inclusion decrepitation, or the presence of cracks that act as fast diffusion pathways.

We thus investigated the diffusion of He in diamond using molecular dynamics (MD) simulations in the Vienna Ab Initio Simulation Package (VASP) at relevant mantle conditions. The density functional theory (DFT) allowed to generate a series of reference structures and MD trajectories. Machine learning techniques were used to fit interatomic potentials on the *ab initio* data, which were refined at each pressure during He diffusion along a mantle adiabat. We employed large simulation boxes exploiting the conventional unit cell of diamond, inside which one He atom was randomly inserted as an interstitial defect. Post-processing analysis of the MD runs was carried out via the Universal Molecular Dynamics package ([2]). Diffusion coefficients as a function of pressure and temperature are reported. The main petrological/geochemical implications are presented and discussed.

[1] Stachel, T., & Luth, R. W. (2015). Diamond formation-Where, when and how? *Lithos*, *220*, 200-220.

[2] R. Caracas, A. Kobsch, N. V. Solomatova, Z. Li, F. Soubiran, J.-A. Hernandez (2021) Analyzing melts and fluids from ab initio molecular dynamics simulations with the UMD package, *JoVE*, e61534.

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