Graphitization in Irradiated Diamonds using Molecular Dynamics

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It is long since known that irradiation of diamonds with sufficient energy results in the breaking of SP3 bonds within the diamond lattice. These damaged areas can, given sufficient broken bonds, be annealed to an amorphous SP2 carbon, or polycrystalline graphite.

It is also known that with enough radiation damage, such diamonds lose their insulation capabilities and begin to act as conductors. It has been hypothesized that such conductance is made possible by percolation of electrons through the damaged areas.

Our study aimed to simulate the generation of graphitic regions in a diamond model, and provide a proof of concept for percolative conductance of electrons.

We heated a diamond model, consisting of several thousand atoms, in several localized areas. Dynamics were done using the Tersoff potential and the Molecular Dynamics code LAMMPS. We then annealed the crystal to allow the formation of graphitic planes, and searched for overlapping areas allowing percolation. An example of such region can be seen in Figure 1. Figure 2 shows the RDF of the corresponding model, with a distinct peak at 1.46 Å, which is the bond length of graphite under the Tersoff potential.

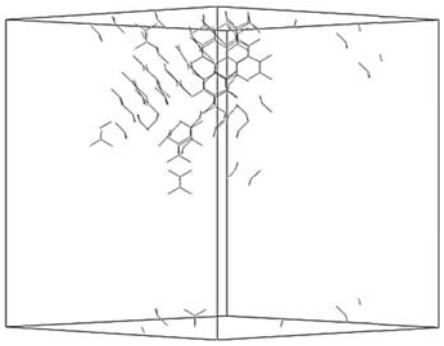

Figure 1: Graphitic Region in Diamond

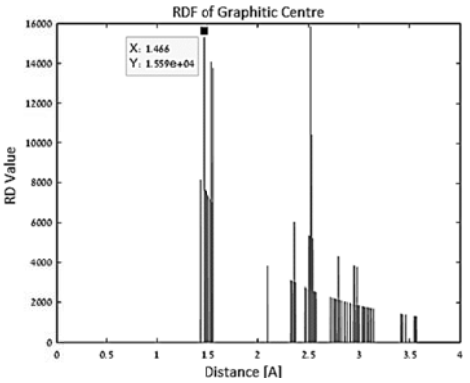

Figure 2: RDF of Damaged Diamond