# XENON IMPLANTATION IN NANODIAMONDS: IN SITU TRANSMISSION ELECTRON MICROSCOPY STUDY AND MOLECULAR DYNAMICS SIMULATIONS.

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**Introduction:** Xenon in nanodiamonds from meteorites is a remarkable impurity. At least two isotopically different components of Xe are known: P3 and Xe-HL. The P3 component might represent adsorbed Xe; whereas the component enriched in heavy and light isotopes (Xe-HL) is likely related to explosions of Supernovae of types I [1] or II [2]. Formation mechanism of nanodiamonds and their astrophysical sources remain debatable. It is widely accepted that the HL component was implanted. However, experimental data on radiation resistance of nanoparticles are scarce and contradictory results were obtained. We present results of the first investigation of the Xe implantation process into nanodiamonds of various sizes studied *in situ* in Transmission Electron Microscope (TEM), complemented by advanced Molecular Dynamics simulations.

**Experiments and modeling:** Several types of nanodiamonds (ND) were studied: NDs extracted from Orgueil meteorite (log-normal size distribution from ~1 to 10 nm with median size around 2.6 nm); synthetic NDs with sizes 4-5 nm with occasional presence of larger particles; synthetic NDs 30-40 nm in diameter. The in situ implantation study was performed at MIAMI facility [3]. Xe ion energies of 6 and 40 keV were employed. The ion energies allowed investigation of various rates of defects introduction by the transmitted ions. Molecular dynamics calculations are performed using completely independent approaches: EDIP and LAMMPS Molecular Dynamics simulator. The environmental dependent interaction potential (EDIP) for carbon in combination with the Ziegler-Biersack-Littmark (ZBL) potential to describe close approaches. The carbon EDIP methodology accurately models the behaviour of disordered and amorphous carbons. In LAMMPS the carbon-carbon interaction was modeled with the Tersoff potential, since it is easy to combine with ZBL to handle large energy interactions. For the Xe-C a Lennard-Jones potential with smooth joint to ZBL at short distances was employed.

**Results:** The most important result of the experiment is that contrary to expectations that nanodiamond grains will gradually amorphise or graphitise, we have observed gradual disappearance of small nanodiamond particles (meteoritic NDs and 4-5 nm synthetic grains) under the beam. The larger grains (>10 nm) were almost unaffected by the ion beam. Such behavior points to existence of a size effect on radiation resistance of carbon nanoparticles.

Molecular dynamics explains the experimental observations with good correlation between the independent modeling approaches. It is shown that the 6 keV Xe ion leads to extreme raise of temperature of a nanodiamond grain, resembling stochastic heating phenomenon usually discussed for UV photons. For the grains ≤2 nm in size the temperature excursions exceed 10000 K which effectively "explodes" the particle. For particles 2-5 nm in size the heating converts the grain to carbon onion-like cluster, though in some cases recrystallisation into diamond structure is also possible. At larger ND grain sizes only points defects are created and since diamond is notoriously resistant to radiation damage [4] the effect of the implantation is not strongly pronounced at fluences employed in the current work. The modeling shows that for the Xe ions the energy of 5-6 keV leads to the most pronounced devastation effect on the smallest particles; at lower energies Xe ions are implanted with formation of some point defects; at higher energies ions are transmitted leaving some damage behind.

Preliminary Monte-Carlo simulations show that qualitatively similar effects could be produced by Kr ions. However, damage levels from light ions such as Si and N which are relevant to studies of meteoritic NDs and for technological applications are always too low to induce such dramatic effects.

**Conclusions:** We demonstrate dramatic influence of nanodiamond grain size on survival of the grains during ion implantation. This work provides tentative explanation of differences in Xe isotopic compositions between different nanodiamonds size fractions [5]. Stochastic heating by ion implantation and/or UV photons might be responsible for preferential observation of the silicon-related defects in the smaller nanodiamond grains [6]. Most likely, these results are not limited to nanodiamonds and have broader astrophysical significance.

**References:**

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