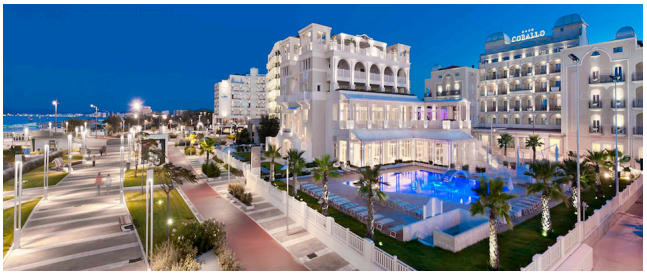

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Impact of Dopant Concentration on the Crystalline Structure of Si-Ge Crystals for the Construction of Crystal-based Light Sources using Molecular Dynamics Simulations

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Crystal-based Light Sources (CLS) offer a novel method to produce sources of gamma-rays. Making use of the channelling phenomena, ultra-relativistic charged particles are directed through bent crystals to produce synchrotron-like radiation. These bent crystals are produced by doping a base crystal, thus changing the crystalline inter-planar distances.

In this preliminary study we conduct molecular dynamics simulations of fixed-sized $Si_{1-x}Ge_x$ crystals doped at Germanium concentrations of $0.00 \leq x \leq 0.30$ and temperatures of 10K and 300K to elucidate the impact of these parameters on the distances between channelling planes.

We observe a linear relationship between Germanium concentration and inter-planar distance, with minimal dependence on temperature at low Germanium concentrations. We observe less formation of crystalline defects than expected from literature. This work will be complemented with experimental characterisations of $Si_{1-x}Ge_x$ crystals.

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