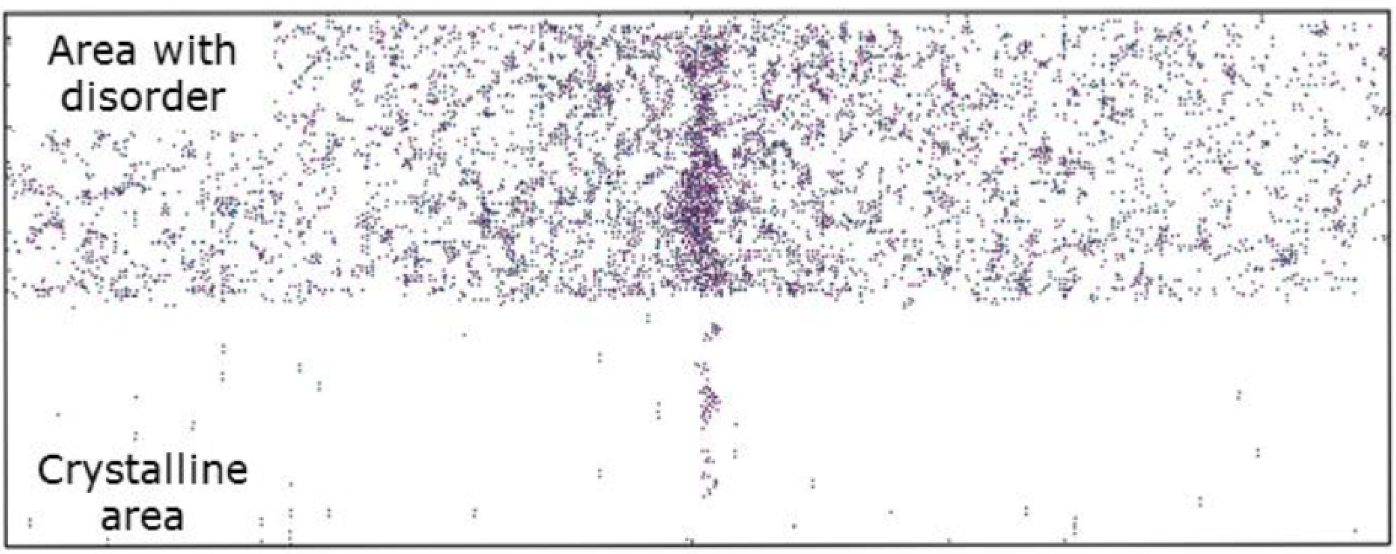
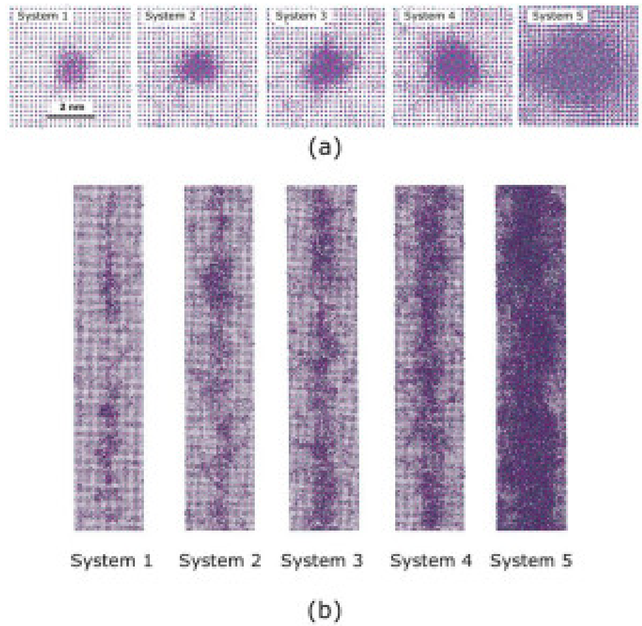
Predictive modeling of ion track formation during irradiation

Radiation is common in nature such as during the decay of radioisotopes in minerals and in space (cosmic radiation), but also in man-made environments, like fusion and fission reactors, nuclear waste disposal facilities, medical imaging and treatment. Ion irradiation is a technique widely used in both industry and research for fabrication, characterization and modification of materials, and creation of nanostructures for various applications, for example in the semiconductor industry. Therefore, fundamental understanding of the interaction of radiation with matter is necessary in order to be able to predict the materials' performance in extreme conditions.
During irradiation, fast moving ions transfer part of their energy to the nuclei of the atoms of the material, and part to the electrons which become excited. The higher the energy of the moving ions, the bigger role the electrons play in the energy transfer from the moving ion to the target material. So, it is important that we understand the role of both the nuclei and the electrons in the materials' behavior during irradiation, not only separately but also together. In our study, we look how the excited electrons affect the energy transfer when the target material is not perfectly crystalline but it already contains some imperfections or disorder.



Using molecular dynamics simulations, in which the atoms are rigid balls and their interactions are described by Newton's equation of motion ??=???, we irradiate samples of strontium titanate ($SrTiO_3$) with different initial disorder using nickel (Ni) ions of 21 MeV energy. While in crystalline systems (zero imperfections) the ions leave no tracks along their path, in the disordered samples the ions leave behind them a track of melted material, which is called an ion track. Depending on how many imperfections exist in the material before the irradiation, the ion tracks have different size and morphology: the more imperfections there are, the larger and more continuous ion tracks are formed. This is a result of the alteration of some of the material's properties because of the presence of the imperfections, such as the way the material conducts heat (thermal conductivity) and the way the excited electrons interact with the lattice vibrations (electron-phonon coupling strength).



These modeling results agree with experimental results that also show a linear relationship of the pre-existing disorder and the ion track diameter size. Our findings highlight a gap in the fundamental knowledge of how the imperfections in a crystal can alter the material's properties, and so they can also alter its behavior under extreme conditions: for intermediate energy ions, ion tracks are formed only in systems with pre-existing disorder and not in perfect crystals. With intermediate energy ions widely available in industry and research, this study opens the way to the exploitation of $SrTiO_3$ ion tracks in material design. Finally, the agreement between simulations and experiments shows (i) the importance of the combination of the two methods for the fundamental understanding of the materials response to radiation and (ii) the importance of modeling as a tool for predicting the materials' performance in a way that is not possible in experiments. Using feedback from simulations, modeling can actually offer guidance in the design of experiments, with benefits in time management and financial planning.

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Publication

Predictive modeling of synergistic effects in nanoscale ion track formation.
Zarkadoula E, Pakarinen OH, Xue H, Zhang Y, Weber WJ
Phys Chem Chem Phys. 2015 Sep 21