THEORETICAL STUDIES OF THE EFFECTS OF GAMMA RADIATION ON PENTAGONAL SILVER NANOWIRES
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Gamma radiation has been widely used in different fields in industry, medicine and investigation. It is known that this type of radiation can cause structural damage to materials, modifying their original properties. With the aim of understanding the consequences of the interaction of gamma radiation with silver nanowires, in this work, we have simulated the behavior of silver nanowires exposed to ionizing radiation at doses of 1, 10 and 20 kGy. The studies of the interaction of gamma radiation with the pentagonal silver nanowires were performed through the Monte Carlo method. Pentagonal silver nanowires of 199 atoms, were constructed and geometrically optimized. The geometric refinement of the atomic structure was performed through an iterative sequence by molecular mechanics to find the stable structures. The SMART algorithm was used to perform these calculations, which is a combination of steps descent methods, conjugate gradient and Newton-Raphson and a Universal potential. The beam direction of the gamma radiation was applied to planes (100) of the silver nanowires and at the intersection between them. After the radiation beam has interacted with the structure, it was observed that structural changes on the silver nanowire might occur and these are dependent of the crystallographic plane where the beam interacted and the dose. These changes correspond mainly to atoms migration from their initial positions, leaving vacancies. As the radiation dose increases, a greater amount of atoms migrate to the surface or is modified from their original positions.

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References:

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