Crack mechanical failure in ceramic materials under ion irradiation: case of lithium niobate crystal.

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Abstract (Arial 10)

Swift heavy ion irradiation (ions with mass heavier than 15 and energy exceeding MeV/amu) transfer their energy mainly to the electronic system with small momentum transfer per collision. Therefore, they produce linear regions (columnar nano-tracks) around the straight ion trajectory, with marked modifications with respect to the virgin material, e.g., phase transition, amorphization, compaction, changes in physical or chemical properties. In the case of crystalline materials the most distinctive feature of swift heavy ion irradiation is the production of amorphous tracks embedded in the crystal. Lithium niobate is a relevant optical material that presents birefringence due to its anysotropic trigonal structure. The amorphous phase is certainly isotropic. In addition, its refractive index exhibits high contrast with those of the crystalline phase. This allows one to fabricate waveguides by swift ion irradiation with important technological relevance. From the mechanical point of view, the inclusion of an amorphous nano-track (with a density 15% lower than that of the crystal) leads to the generation of important stress/strain fields around the track. Eventually these fields are the origin of crack formation with fatal consequences for the integrity of the samples and the viability of the method for nano-track formation. For certain crystal cuts (X and Y), these fields are clearly anisotropic due to the crystal anisotropy.

We have used finite element methods to calculate the stress/strain fields that appear around the ion-generated amorphous nano-tracks for a variety of ion energies and doses. A very remarkable feature for X cut-samples is that the maximum shear stress appears on preferential planes that form +/-45º with respect to the crystallographic planes. This leads to the generation of oriented surface cracks when the dose increases. The growth of the cracks along the anisotropic crystal has been studied by means of novel extended finite element methods, which include cracks as discontinuities. In this way we can study how the length and depth of a crack evolves as function of the ion dose. In this work we will show how the simulations compare with experiments and their application in materials modification by ion irradiation.