ION-BEAM DAMAGE AND NON-RADIATIVE EXCITON DECAY IN LiNbO_3

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It is well documented¹ that ionizing radiation (electrons, X-rays, UV light) produces intrinsic Frenkel pairs in alkali halide crystals via non-radiative decay of self-trapped excitons at X_2^- sites (X being an anion). On the other hand, it is generally believed that energetic ions cause atomic displacements and lattice damage through nuclear collisions. However, there is evidence that, during ion bombardment, electronic excitation processes induce damage and even amorphization in LiNbO_3 and many other oxides. This type of damage presents a number of differential features in comparison to that associated to nuclear collisions. In particular, a threshold value for the electronic stopping power (or deposited energy density) should be reached to cause observable damage. In this work, following a suggestion made by Itoh², we develop a non-radiative exciton decay model to account for defect formation. It is based on the existence of self-trapped excitons i.e. O^- holes trapped at small polarons Nb^{+4} . It is proposed that the decay of these excitons may proceed either by light emission or non-radiative molecular dissociation. The key point is that the adiabatic potential energy surface (APES) for the excited state presents an energy barrier separating the bound and dissociated states. The high temperature reached at the thermal spike generated by the bombarding ion provides the necessary activation energy. Here, we explore such a model and describe quantitatively the rate of light emission and defect formation. The predictions of the model satisfactorily account for the results found under single impact as well as multiple impact irradiation. Some theoretical predictions requiring experimental confirmation are advanced.

1. F. Agulló-López, R.C. Catlow, and P.D. Townsend, *Point Defects in Materials*, Academic Press, London, 1984.

2. N. Itoh, Nucl. Instrum. Meth. **B 135**, 175 (1998).