

Rezumat stiintific al rezultatelor obtinute in ETAPA II (2022): Obiectivul principal al acestei etape a fost investigarea evolutiei defectelor preexistente in KTaO_3 (create in urma iradierii cu ioni grei, 2 MeV Au) in functie de pierderea de energie electronică (S_e) a ionilor de energie medie (5 MeV C, 7 MeV Si, 12 MeV O). Prin explorarea acestor procese in KTaO_3 , rezultatele experimentale si teoretice au demonstrat ca, pentru un nivel initial de dezordine (f_0) de aproximativ 0.3 si pentru valori ale $S_e \geq 4.65 \text{ keV/nm}$ (7 MeV Si), efectul sinergistic este activ. Acest efect induce crearea de nano-canale („ion tracks”). La valori mai mici ale S_e (5 MeV C si 12 MeV O), cresteri minore ale f_0 sunt observate initial la o fluență ionică de 10 ioni/ nm^2 . Acest fenomen poate fi atribuit provizoriu dizolvării clusterelor interstițiale sau amorse preexistente. Pe de altă parte, odată cu creșterea suplimentară a fluenței de ^{12}C sau ^{16}O (de la 10 la 20 ioni/ nm^2), se observă o tranzitie de la producția de defecte la procesul de recristalizare atermică responsabil de anihilarea defectelor, procese ce nu au fost raportate anterior in KTaO_3 .

Scientific summary of the results obtained in 2022: Understanding the inelastic interactions of ions with defective KTaO_3 may provide nonequilibrium pathways to tune the functional properties of this perovskite. In this regard, defective KTaO_3 has been irradiated with several ion species (5 MeV C, 7 MeV Si, 12 MeV O and 18 MeV Si ions) over an extended selection of ion fluences at 300 K. By exploring these processes in KTaO_3 , the experimental characterization and computer simulations show that, for a pre-damaged fractional disorder level of 0.3 and $S_e \geq 4.65 \text{ keV/nm}$ (7 MeV Si ions), the synergistic effect is active, which enables ion track creation under these conditions [1,2]. In additions, we further reveal that the size of these latent ion tracks increases with S_e and level of pre-existing damage [1]. For $S_e \leq 3.03 \text{ keV/nm}$ (5 MeV C and 12 MeV O), minor increases in disorder are observed initially over a region of depth at an ion fluence of 10 ions/ nm^2 , which may be triggered by the dissolution of pre-existing interstitial or amorphous clusters; surprisingly, with further increase in ion fluence, a ionization-induced damage recovery processes is observed [2]. These findings reveal a competitive two-stage phase transition process that leads to damage recovery process, not previously reported in KTaO_3 .

- [1] G. Velișa, E. Zarkadoula, D. Iancu, M.D. Mihai, C. Grygiel, I. Monnet, B. Kombaiah, Y. Zhang, W.J. Weber, Near-surface modification of defective KTaO_3 by ionizing ion irradiation, *J. Phys. D: Appl. Phys.* 54 (2021) 375302. doi:10.1088/1361-6463/AC0B11.
- [2] D. Iancu, E. Zarkadoula, M.D. Mihai, C. Burducea, I. Burducea, M. Straticiuc, Y. Zhang, W.J. Weber, G. Velișa, Revealing two-stage phase transition process in defective KTaO_3 under inelastic interactions, *Scr. Mater.* 222 (2023) 115032. doi:10.1016/J.SCRIPTAMAT.2022.115032.

Graphical Abstract

