Supplementary Information

Localized thermal spike driven morphology and electronic structure transformation in swift heavy ion irradiated TiO_2nanorods

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Table T1. Some of the important published works on Ag ion irradiation effects on TiO_2

Material (Reference)	Ion/Energy/Fluence	Study on/observed phenomena
Undoped and niobium doped anatase TiO_2 thin film[1]	120 MeV Agand 130 MeV Ni ions at different ion fluence of 5×10^{11},1×10^{12}, 3×10^{12} and 1×10^{13} ions/cm^2	A study on phase transformation
Rutile TiO_2 thin film[2]	120 MeV Ag ions at fluences from1×10^{11} to 2×10^{13} ions/cm^2	Micro-Raman study
Amorphous TiO_2 thin films[3]	100 MeV Ag ion beam at a fluences of 1×10^{12} and 1×10^{13} ions/cm^2.	Rapid thermal annealing effect on SHI induced nanocrystalline thin film
Anatase TiO_2 thin film[4]	200 MeV Agions at fluences of 1×10^{11}, 1×10^{12}, and 5×10^{12} ions/cm^2	Transition from anatase to a mixed phase of brookite and rutile; changes in electronic structure observed by XAS study
Amorphous	200 MeV Ag ion at fluences from 5 ×	A comparative study of thermal annealing and

TiO_2thin film[5]	10^{11} to 3×10^{12} ions/cm^2	SHI induced structural evolution. SHI leads to a structural evolution from anatase phase to pure rutile
Amorphous TiO_2 thin film[6]	100 MeV Ag ion beam at fluences of 1×10^{12} and 1×10^{13} ions/cm^2	Formation of nano-hillocks, amorphous to crystalline phase transition
Amorphous TiO_2 thin film[7]	100MeV Ag ion at a fluence of 1×10^{12}ions/cm^2	Nano crystallization of amorphous thin film, the amorphous unirradiatedPLD film containing small amount of rutile phase isrecrystallized toanatasephase after SHI irradiation

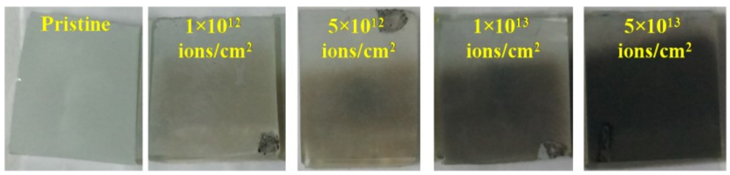

Fig. S1. Digital photographs of pristine and irradiated samples at different fluences

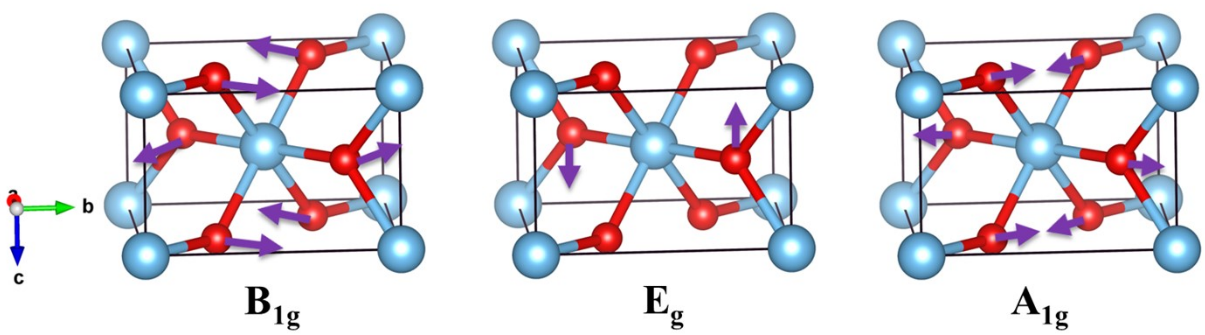

Fig. S2. Schematic of the vibrations of oxygen atoms corresponding to Raman modes in rutile TiO_2.[8] The Ti and O atoms are represented by light blue and red solid spheres, respectively.

Ion energy selection

To estimate the electronic/inelastic (S_e) and nuclear/elastic (S_n) energy loss by the incident ion beam, simulations based on SRIM code[9] were executed, and the results are presented in Fig.S3. It is observed from Fig.S3(a) that S_e dominates in the incident energy range upto 10^3 MeV with a maximum value at around 300 MeV. However, for 100 MeV Ag ions interacting with TiO_2, the value of S_e is 19.82 keV/nm, which is more than two orders of magnitude higher than the S_n (0.09 keV/nm). The S_e and S_n values of the 100 MeV Ag ion along the depth inside TiO_2 are presented in Fig.S3(b). It is observed that the S_e and $S_n$values remain almost constant along the depth (1 μm long TiO_2nanorods as observed in SEM images).

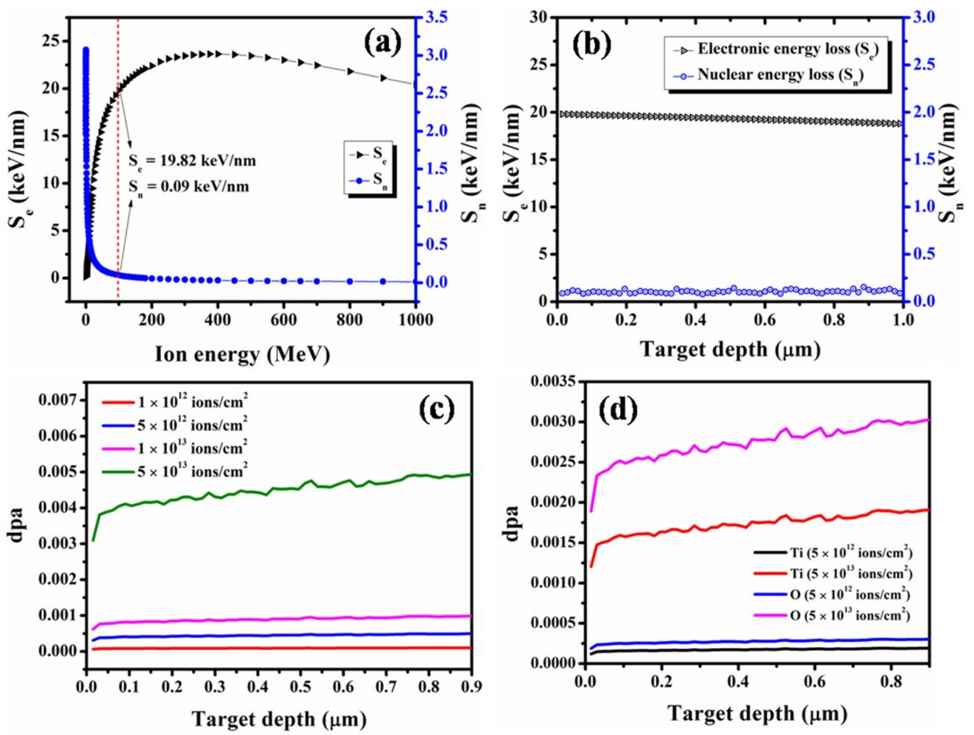

Fig.S3. (a) Electronic/inelastic (S_e) and nuclear/elastic (S_n) energy losses in TiO_2 as a function of incident Ag ion energy, (b) the depth profile of S_e and S_n in TiO_2 irradiated with 100 MeV Ag ion simulated with the SRIM 2013 code,[9] (c) total vacancies per volume,and (d) the titanium and oxygen vacancies per volume along the depth at different fluencesof 100 MeV Ag ion irradiationestimated using TRIM full cascade simulation.[9]

The number of vacancies created at different fluences was also estimated from TRIM full cascade simulation.[9] This was expressed as the ratio of the number of atoms displaced over the total number of atoms in a certain volume of TiO_2. Fig.S3(c) presents the displacement per atom (*dpa*) along the length of the nanorod, which shows a gradual increment in the vacancy distribution with increasing fluence along with a stable depth profile. The estimation reveals a *dpa* of 0.005 representing 5 vacancies per 1000 atoms created in TiO_2 at the highest fluence of 5 $\times 10^{13}$ ions/cm^2. TRIM simulation also demonstrated a higher concentration of oxygen vacancies compared to that of titanium, which is presented in Fig. S3(d).

Table T2. Physical parameters of rutileTiO_2 for i-TS calculation

Parameters	**Values for rutile TiO_2**[10,11,12]
Density for solid (g/cm^3)	4.25
Density for liquid (g/cm^3)	3.21
Specific heat of electron (J/cm^3.K)	1
Thermal conductivity of electron (J/cm K sec)	2
Specific heat of lattice (J/g.K)	$C_a(T) = 0.96072 - 1.15732 \times e^{(-0.00482 \times T)}$
Thermal conductivity of lattice (J/cm K sec)	$K_a(T) = 0.03215 + 0.2836 \times e^{(-T/200)}$
Latent heat of fusion (J/g)	838.07
Melting point (T_m) in K	2130
Latent heat of vaporization (J/g)	6157.0
Boiling point (T_b) in K	3200
Electron-phonon mean free path (nm)	5.8

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