

Supporting Information

Influence of defects on linear and nonlinear optical properties of Cu doped rutile TiO₂ microflowers

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The crystallite size (D) of undoped and Cu doped TiO₂ is calculated using Debye–Scherrer’s formula as given below

$$D = \frac{0.9 \lambda}{\beta \cos \theta} \quad (1)$$

Where, D is the crystallite size, λ is the wavelength of incident X-ray (1.5418 Å), β is the full-width half maxima (FWHM) in radian and θ is the angle of diffraction.

The dislocation density is calculated using the relation,

$$\delta = \frac{1}{D^2} \quad (2)$$

Further by using the Bragg’s diffraction law as shown in equation (4), the value of d_{110} is calculated and presented in Table S1.

$$2d \sin \theta = n \lambda \quad (3)$$

The value of d_{110} and the equation (5) is used for the calculation of lattice parameter “a”. As rutile TiO₂ has a tetragonal structure, “a”=”b”.

Similarly, d_{101} is calculated using 101 peak. The value of “c” is obtained by using lattice parameter “a” and d_{101} .

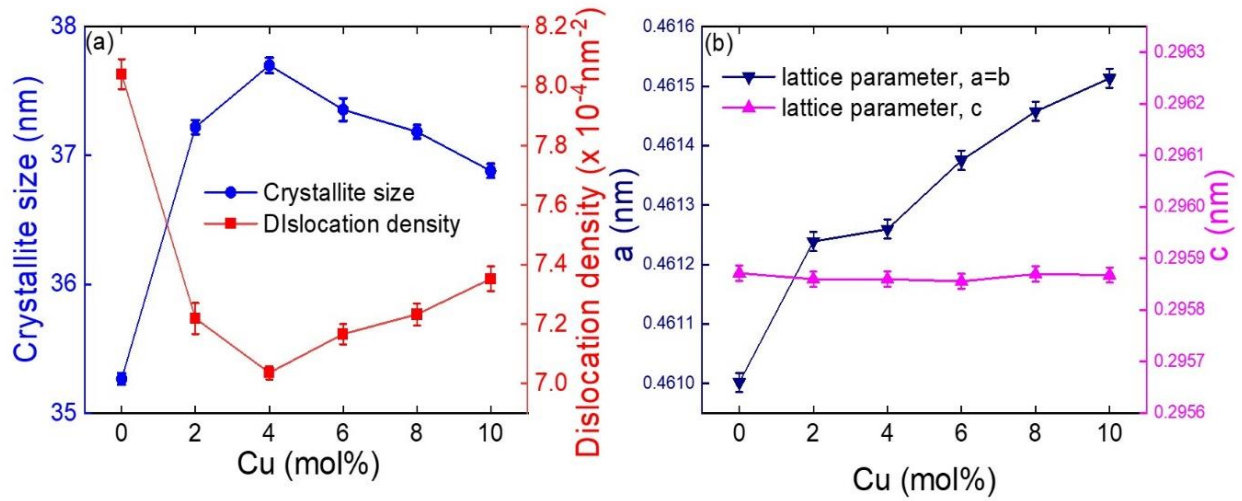


Figure S1: (a) Variation of crystallite size (left side) and dislocation density (right side) with Cu concentration. (b) Variation of lattice parameter with Cu concentration.

The value of microstrain (ϵ), calculated using the relation is obtained using equation (3), the lattice parameters (a=b, c) are presented in Table 1.

$$\epsilon = \frac{\beta}{4 \tan \theta} \quad (4)$$

Table S1: Values of interplanar spacing d_{110} and microstrain for undoped and Cu doped TiO_2 .

Samples	d_{110} (nm)	microstrain
Undoped TiO_2	0.32602	0.004113
2% Cu: TiO_2	0.32619	0.004114
4% Cu: TiO_2	0.32620	0.004116
6% Cu: TiO_2	0.32629	0.004121
8% Cu: TiO_2	0.32634	0.004132
10% Cu: TiO_2	0.32638	0.004135

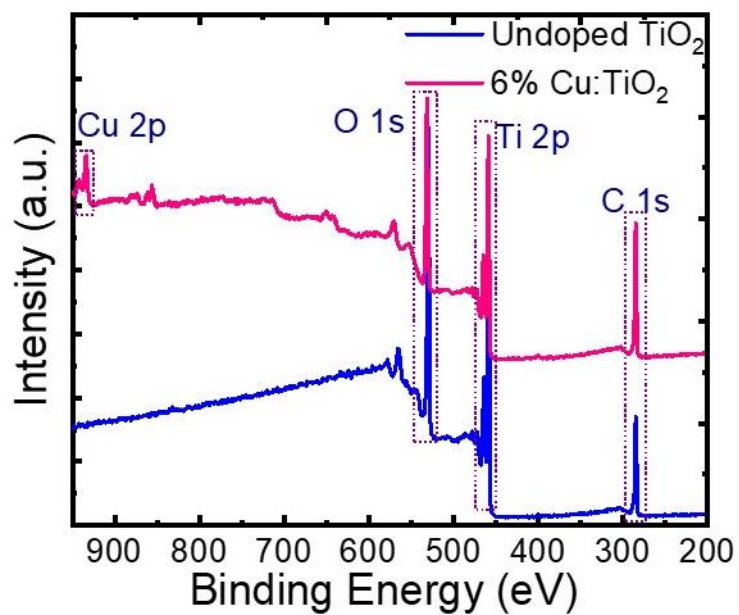


Figure S2: XPS survey spectra of undoped and 6% Cu doped TiO₂

Table S2: %Area of the peaks

Peak	Undoped TiO ₂	6% Cu doped TiO ₂
529.59	80.84	68.65
530.71	7.63	9.97
531.56	8.66	16.47
532.49	2.86	4.90