Electronic Supplementary Material

Study of effect of chromium on titanium dioxide phase transformation by A Bellifa (pp 669–677).

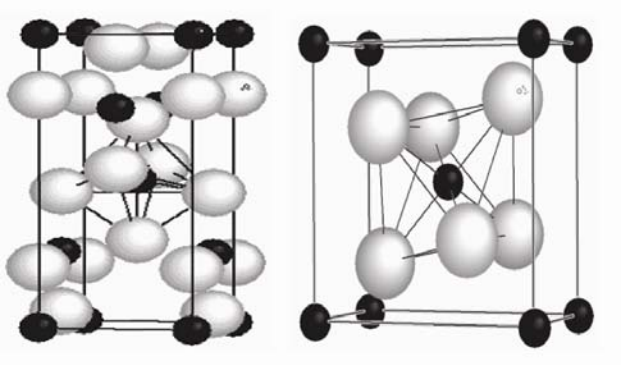


Figure S1. Structural schemes of anatase to rutile transition.

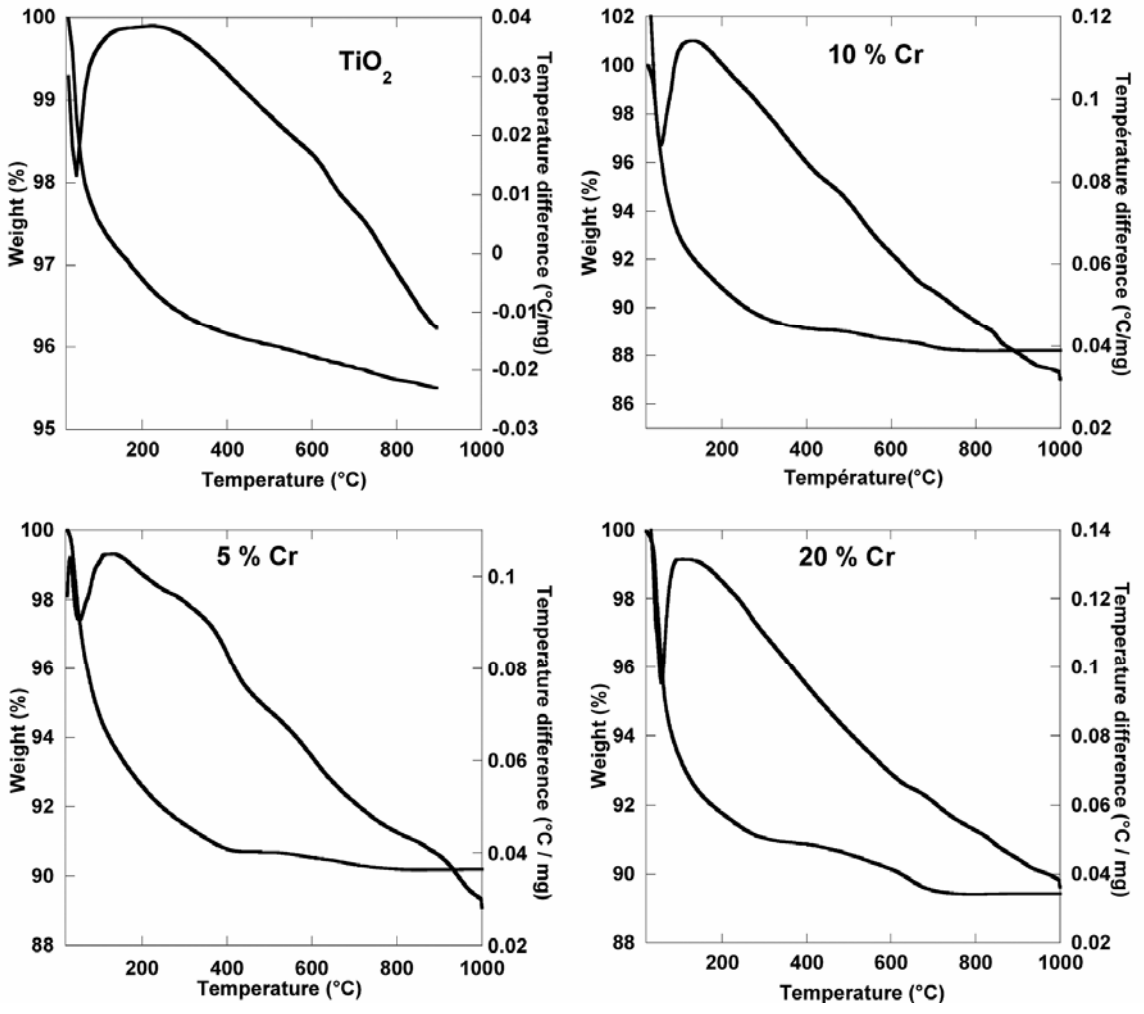


Figure S2. Analysis ATG-ATD for different samples.

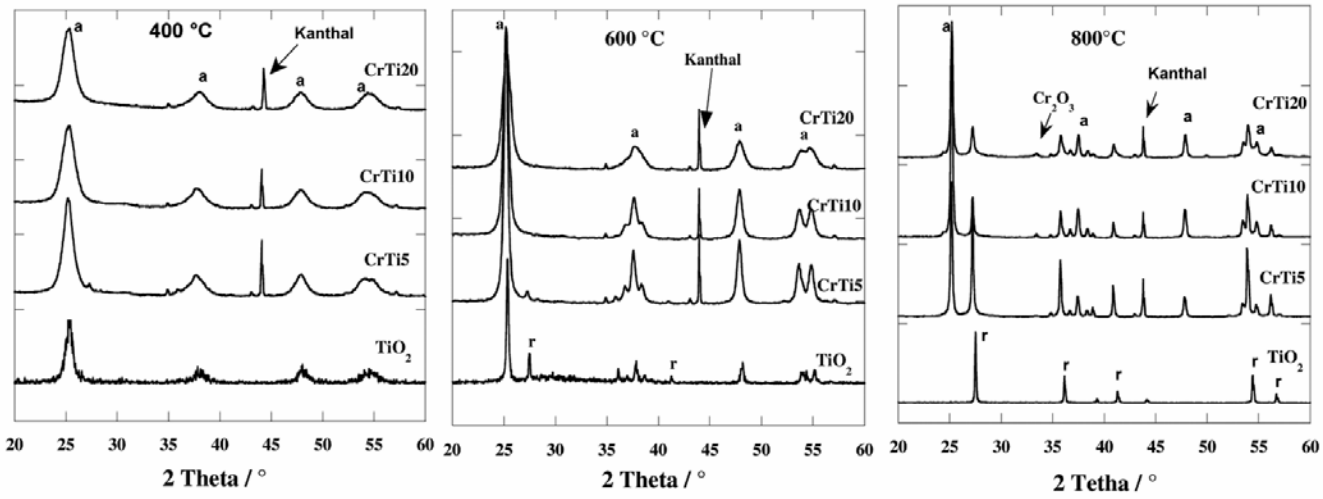


Figure S3. *In situ* XRD diffractograms of CrTiX; a: anatase, r: rutile.

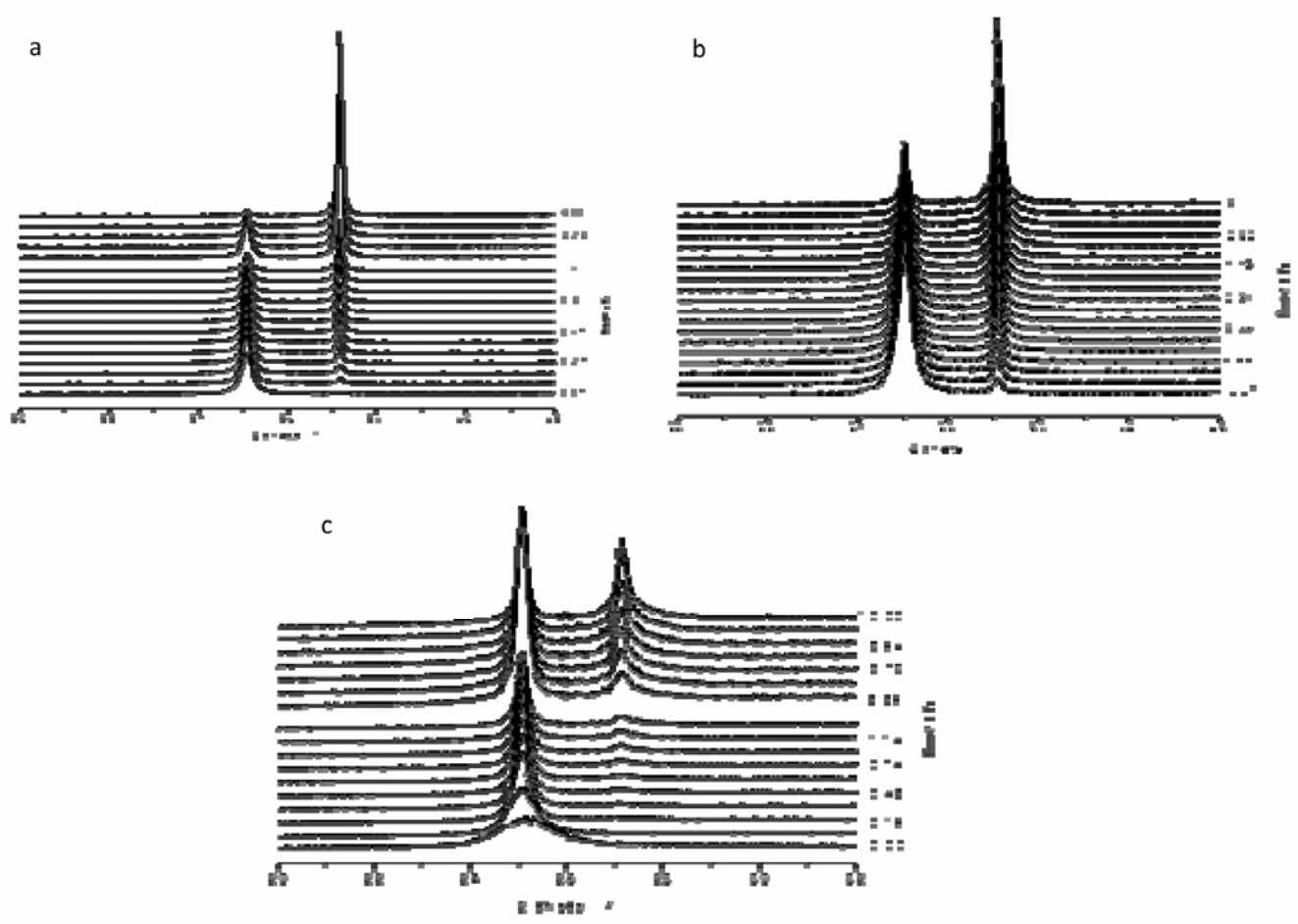


Figure S4. XRD diffractograms of anatase-rutile transition vs time: (a) TiO_2 at 650 °C, (b) $CrTi_5$ at 750 °C and (c) $CrTi_{20}$ at 750 °C.

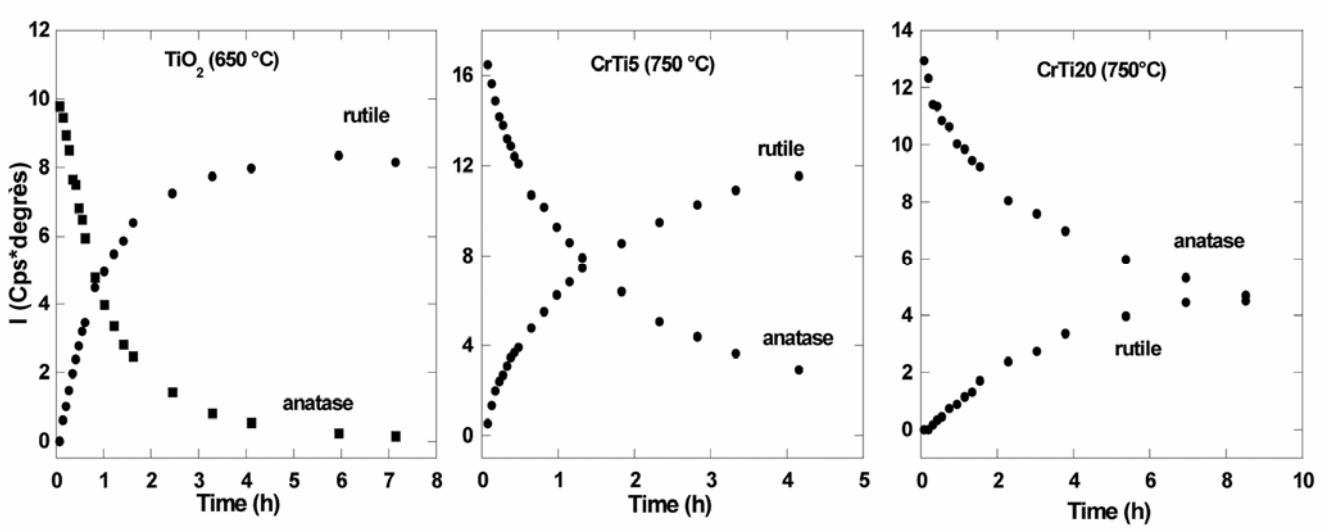


Figure S5. Evolution of anatase and rutile phase vs time.

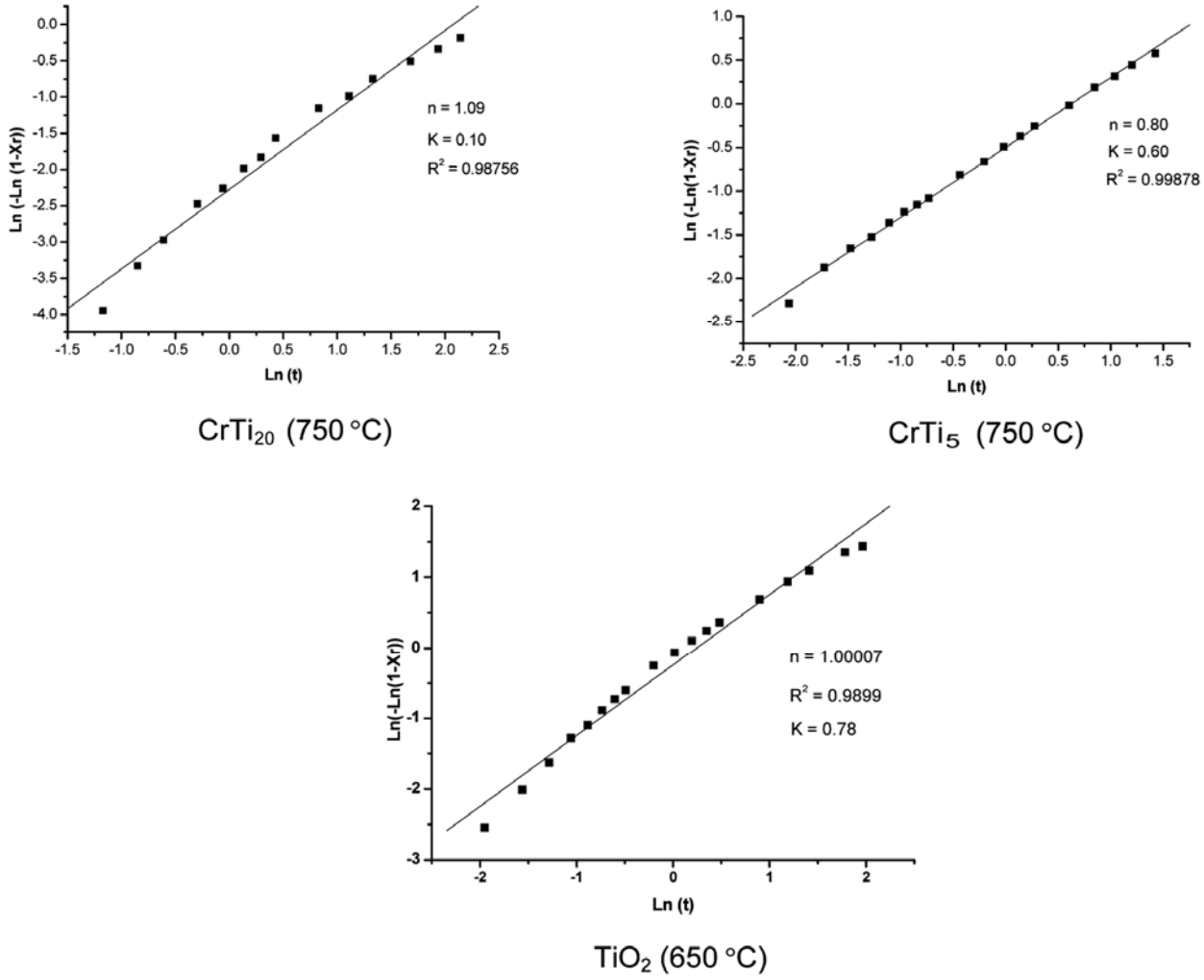


Figure S6. Avrami plot.

Table S1. Physical, chemical and structural parameters of anatase, brookite and rutile phases.

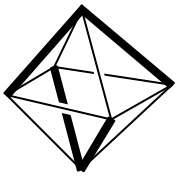
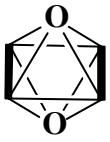
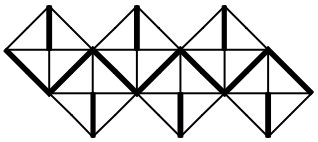
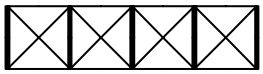
Parameters	Anatase	Brookite	Rutile
PDF ref.	21–1272	29–1360	21–1276
Space group	Tetragonal	Orthorhombic	tetragonal
	$I4_1/amd$ (141)	*Pcab* (61)	$P4_2/mnm$ (136)
Parameters	a = 3·78520	a = 5·45580	a = 4·59330
	c = 9·51390	b = 9·18190	c = 2·95920
		c = 5·14290	
Z	4	8	2
Volume ($Å^3 \cdot (TiO_2)^{-1}$)	34·078	32·204	31·215
Density ($g \cdot cm^{-3}$)	3·893	4·120	4·250
$\Delta_f H°$ (298) ($kJ \cdot mol^{-1}$)	–941·40		–944·75
$S°$ (298) ($J \cdot K^{-1} \cdot mol^{-1}$)	49·907		50·292
Melting point (°C)	1676		1843
Ti–O (Å)	4 × 1·9341; 2 × 1·9798	1·87 to 2·04	4 × 1·9486; 2 × 1·9799
Octahedral packing	2 × 2 shared edges	3 shared edges	2 parallel shared edges
	8 free edges	4 corners	2 corners
		5 free edges	10 free edges
			
Coordination scheme			
Ti–Ti (Å)	4 × 3·0396 (tetra)		2 × 2·9592 (linear)
	4 × 3·7852 (square)		8 × 3·5691 (cell)
	8 × 5·4582 (cell)		4 × 4·5933 (square)

Table S2. Surface area, porous volume and pore size of the samples.

Sample	S_{BET} ($m^2 \cdot g^{-1}$)	Pore volume ($cm^3 \cdot g^{-1}$)	Average pore size (nm)	S_{XRD} ($m^2 \cdot g^{-1}$)
TiO_2	68	0·06	3·60	154
$CrTi_5$	180	0·22	5·00	220
$CrTi_{10}$	230	0·19	3·30	257
$CrTi_{20}$	152	0·10	2·60	257

Samples calcined at 400 °C.

Table S3. Phase composition and crystallite size (in parenthesis (nm)) vs temperature.

	TiO_2		CrTi5		CrTi10		CrTi20	
T (°C)	*%A*	*%R*	*%A*	*%R*	*%A*	*%R*	*%A*	*%R*
400	100(10)	0	100 (07)	0	100(06)	0	100(06)	0
500	100(16)	0	100 (10)	0	100(13)	0	100(07)	0
600	85(27)	15(41)	100 (16)	0	100(13)	0	100(09)	0
700	2(37)	98(36)	97(22)	3(32)	100(22)	0	100(20)	0
800	0	100(40)	53(32)	47(37)	82(32)	18(39)	88(30)	12(35)

A: anatase; *R*: rutile; *T*: temperature.