# Computational Materials Physics

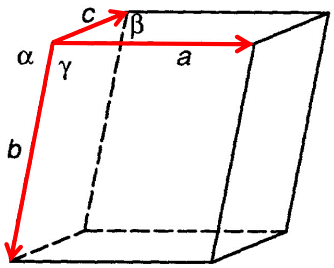
Center for Molecular Modeling

Department of Materials Science and Engineering

## what's in a cif ?

Stefaan.Cottenier@ugent.be
Technologiepark 903, Zwijnaarde

http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs




γ is the angle between *a* and *b*
β is the angle between *a* and *c*
α is the angle between *b* and *c*

Materials science

**The hardest known oxide**

L. S. Dubrovinsky*, N. A. Dubrovinskaia*, V. Swamy†, J. Muscat†, N. M. Harrison‡, R. Ahuja§, B. Holm§, B. Johansson§||

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page 653

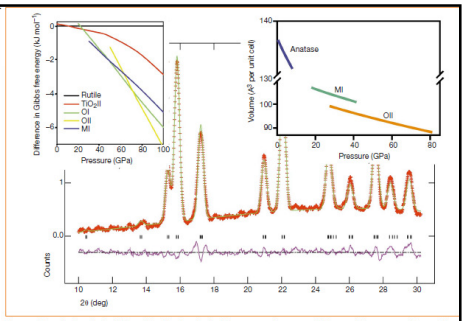
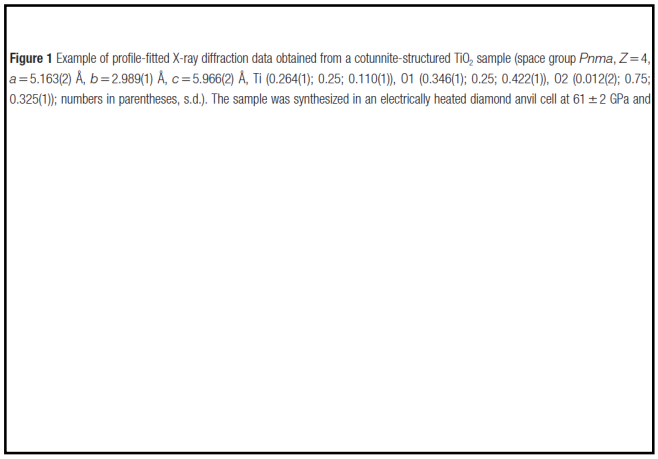



**Figure 1** Example of profile-fitted X-ray diffraction data obtained from a cotunnite-structured $TiO_2$ sample (space group *Pnma*, $Z = 4$, $a = 5.163(2)$ Å, $b = 2.989(1)$ Å, $c = 5.966(2)$ Å, Ti (0.264(1); 0.25; 0.110(1)), O1 (0.346(1); 0.25; 0.422(1)), O2 (0.012(2); 0.75; 0.325(1)); numbers in parentheses, s.d.). The sample was synthesized in an electrically heated diamond anvil cell at 61 ± 2 GPa and 1,100 ± 25 K and then temperature-quenched to 290 K. The GSAS program[12] was used in Rietveld refinement[12] ($wR_p = 1.9\%$, $R_p = 1.6\%$, $\chi^2 = 0.49$). Left inset shows the stability of various known and hypothetical $TiO_2$ polymorphs relative to rutile as a function of pressure, obtained by lattice dynamics at $T = 300$ K; right inset shows the pressure dependence of the volume for the anatase, baddeleyite and cotunnite phases of $TiO_2$. Birch–Murnaghan equations of state are plotted as solid lines, with parameters $K_{300} = 178 \pm 1$ GPa, $K' = 4$ (fixed) and $V_0 = 20.59 \pm 1$ cm$^3$ mol$^{-1}$ for anatase; $K_{300} = 304 \pm 6$ GPa, $K' = 3.9 \pm 2$ and $V_0 = 16.90 \pm 3$ cm$^3$ mol$^{-1}$ for baddeleyite type; and $K_{300} = 431 \pm 10$ GPa, $K' = 1.35 \pm 10$ and $V_0 = 15.82 \pm 3$ cm$^3$ mol$^{-1}$ for the cotunnite type (OII) phase.



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more information on how to make your own cif files with VNL :

http://docs.quantumwise.com/tutorials/cif/cif.html