Computational Materials Physics

Center for Molecular Modeling

Department of Materials Science and Engineering

a "hard" example

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

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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A material as hard as diamond or cubic boron nitride has yet to be identified[1–6], but here we report the discovery of a cotunnite-structured titanium oxide which represents the hardest oxide known. This is a new polymorph of titanium dioxide, where titanium is nine-coordinated to oxygen in the cotunnite ($PbCl_2$) structure.

Table 1 Hardness of polycrystalline materials

Material	Bulk modulus (GPa)	Hardness* (GPa)	Ref.
B_4C	200	30 (30)	3
SiC	248	29 (29)	3
Al_2O_3	252	20 (19)	7
SiO_2, stishovite	291	32 (33)	7
WC	421	30 (30)	8
Cubic BN	369	(32)	3
Cotunnite-type TiO_2†	431	38	
Sintered diamond	444	(50)	3

*Literature data are given in parentheses. The uncertainty in measured hardness is less than 3 GPa.
†Measurements were made at 157 ± 2 K.

Calculate yourself, using crystal info on next slide

By now, you know what this means !

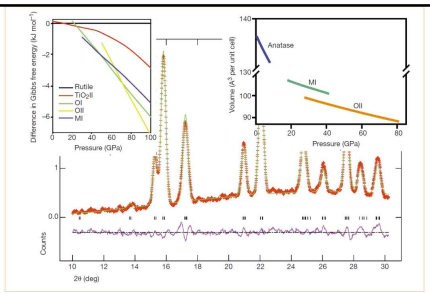

Figure 1 Example of profile-fitted X-ray diffraction data obtained from a columnite-structured TiO_2 sample (space group *Pnma*, $Z = 4$, $a = 5.163(2)$ Å, $b = 2.989(1)$ Å, $c = 5.966(2)$ Å, Ti (0.264(1); 0.25; 0.110(1)), O1 (0.346(1); 0.25; 0.422(1)), O2 (0.012(2); 0.75; 0.325(1)); numbers in parentheses, 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] ($wR_p = 1.9\%$, $R_F = 1.6\%$, $\chi^2 = 0.49$). 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.