

around 1.5 eV binding energy. When crossing the MIT (140 K, antiferromagnetic insulating (AFI) phase), the coherent peak disappears and one observes the opening of a gap of 220 ± 20 meV. Calculations performed for various values of the parameter U , find that $U = 4.2$ eV provides the best simultaneous description of the various phases observed in V_2O_3 . Large values of U result in the opening of another gap for the structure corresponding to the metallic phase. Panel (b) and (c) show PES spectra compared to LDA+DMFT calculations. In the metallic phase (panel b) the agreement is remarkably good, where the calculation matches simultaneously the ratio between coherent and incoherent parts as well as their location on the energy scale. In the insulating phase (panel c), calculations give the correct energy position of the intensity maximum but, even using an increased broadening (0.6 eV), the agreement remains qualitative. The experimental intensity spreads over a larger bandwidth than in the calculations. At present, we have no explanation for such difference.

Figure 2 compares the intensity of the coherent quasiparticle peaks at E_f (inset) and of the V $2p_{3/2}$ shake down satellite for two sample preparations (flat surface area and rough surface). We observe that the presence of the core level satellites is directly related to the

valence band coherent peaks, and that macroscopic imperfections (sample 2) depress both the satellite intensity and the coherent intensity at E_f .

Our results not only confirm the remarkable change of the screening properties in TMO when going from the surface to the volume, but open the way to the determination of important parameters such as the on-site Coulomb interaction via the combined analysis of core level and valence band PES spectra.

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Principal Publication and Authors

G. Panaccione (a), M. Altarelli (b), A. Fondacaro (c), A. Georges (d), S. Huotari (c), P. Lacovig (e), A. Lichtenstein (f), P. Metcalf (g), G. Monaco (c), F. Offi (h), L. Paolasini (c), A. Poteryaev (d), O. Tjernberg (k), M. Sacchi (i), *Phys. Rev. Lett.* **97**, 116401 (2006).

(a) TASC Laboratory, INFN - CNR, Trieste (Italy)

(b) European XFEL Project c/o DESY, Hamburg (Germany)

(c) ESRF

(d) Ecole Polytechnique, Palaiseau (France)

(e) Sincrotrone Trieste (Italy)

(f) Inst. für Theoretische Physik, Univ. Hamburg (Germany)

(g) Dep. of Chemistry, Purdue University, West Lafayette (USA)

(h) Dip. di Fisica Univ. Roma III (Italy)

(k) LMSP, Royal Institute of Technology, Kista (Sweden)

(i) LCP-MR, Univ. P. et M. Curie, Paris, and Synchrotron SOLEIL, Gif-sur-Yvette (France)

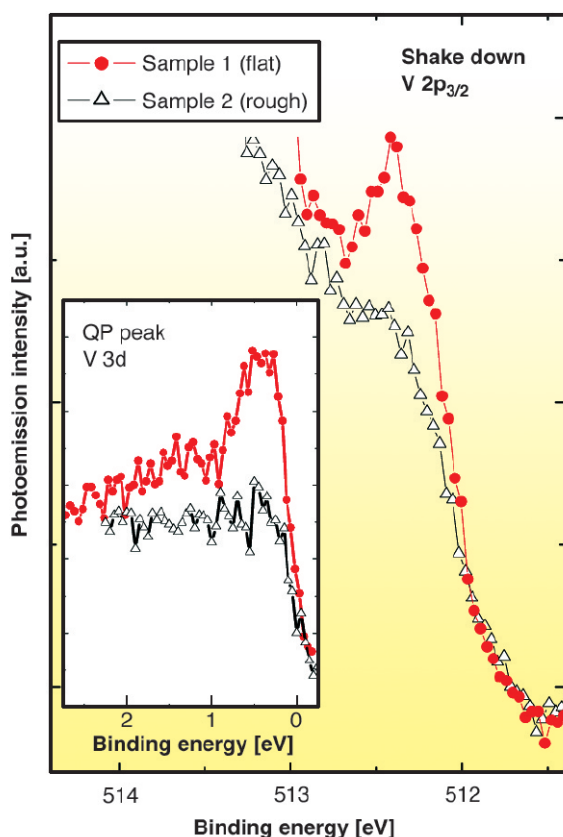


Fig. 2: Room temperature V $2p_{3/2}$ core-level and (inset) valence band for two different samples preparations: cleaved flat surface (red circles) and mechanically polished rough surface (open triangles). The spectra have been arbitrarily scaled by a multiplication factor for better comparison.

Observing the high-frequency limit of sound waves in glasses

Glasses, like all condensed phases, essentially behave as elastic continua for sound waves of sufficiently low frequencies. These can be described by plane waves with well defined wave vector q , related to the angular frequency Ω by $\Omega = vq$, where v is the phase velocity of sound. These waves propagate with an energy mean free path l . Two principal mechanisms produce a finite l in insulating glasses: the relaxation of defects and the anharmonic coupling with modes of the thermal bath, as recently reanalysed in [1]. The question of interest here is what happens at frequencies sufficiently high to probe

the intrinsic structural or dynamical inhomogeneities of glasses. Can these produce such a high attenuation that acoustic excitations lose their wavelike character, as suggested by observations of low-temperature thermal conductivities?

The corresponding frequencies became accessible thanks to Brillouin X-ray scattering on ID16. **Figure 1** shows Brillouin linewidths, $\Gamma \equiv v/l$, obtained on two oxide glasses, permanently densified silica (d -SiO₂) [2] and lithium diborate (LB2). In both cases, a dramatic increase of Γ , approximately $\propto \Omega^4$, is observed up to the frequencies Ω_{IR} shown by arrows at $\Gamma = \Omega/\pi$. The latter implies that l decreased to half the sound wavelength. Thus, Ω_{IR} corresponds to the Ioffe-Regel (IR) crossover beyond which plane waves cease to be a useful concept. One should remark that although similar onsets of crossover are observed for these two glasses at $\Omega/2\pi$ in the THz range, the linewidths behave quite differently at lower frequencies. LB2 reveals a $\Gamma \propto \Omega^1$ dependence in Brillouin light scattering, characteristic of the thermal relaxation of defects, while d -SiO₂ is dominated by anharmonicity, leading to $\Gamma \propto \Omega^2$ [1].

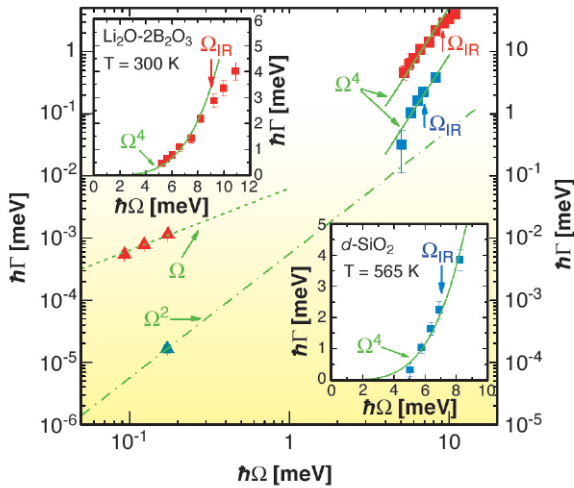


Fig. 1: Brillouin scattering linewidths observed with visible light (▲) and X-rays (■). Note that for clarity the two ordinate scales are distinct as indicated by colours. The insets show the same X-ray data on linear scales, emphasising the rapid onset and the smallness of the error bars, where blue symbols are for d -SiO₂ and red symbols for lithium diborate. The lines are explained in the text.

It is well known that most glasses also exhibit an excess of modes in their reduced vibrational density of states, $Z(\omega)/\omega^2$, peaking at a relatively low frequency Ω_{BP} , called the boson peak. It is remarkable that $\Omega_{IR} \approx \Omega_{BP}$ for the two glasses of **Figure 1**. This is presumably not an accident. It suggests that the IR-crossover indeed results from the hybridisation of acoustic excitations with excess ones, as recently described in [3]. As shown there, this hybridisation should lead to $\Gamma \propto \Omega^4$ below Ω_{IR} . However, for most glasses, Ω_{BP} is lower than in the

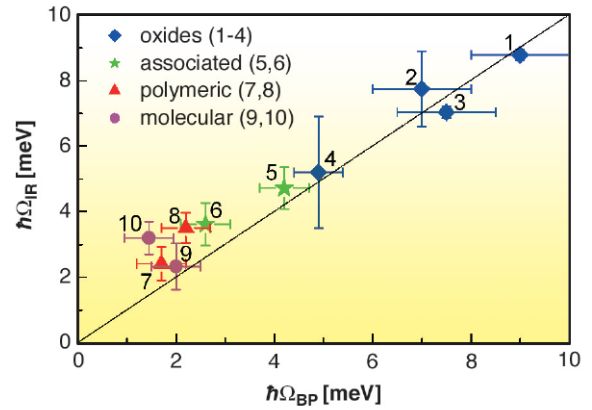


Fig. 2: Relation between Ω_{IR} and Ω_{BP} from literature data. The points are: (1) LB2 at 573 K; (2) lithium tetraborate $\text{Li}_2\text{O}-4\text{B}_2\text{O}_3$ at 600 K; (3) densified silica at 565 K; (4) vitreous silica at 1050 K; (5) glycerol at 175 K; (6) ethanol at 86 K; (7) selenium at 295 K; (8) polybutadiene at 140 K; (9) propylene carbonate at 167 K ($T_g + 7$ K); (10) orthoterphenyl at 156 K. The line is a guide to the eye. See ref. [3] for references to the experimental data.

experimentally favourable cases of d -SiO₂ and LB2. This generally leads to scattering vectors at the IR-crossover that fall near the lower limit attainable with the current spectrometers. It is thus understandable that the onset region $\Gamma \propto \Omega^4$ was so far not observed in other glasses. However, there is now sufficient information in the literature to extract good estimates and error bars for Ω_{IR} in a number of cases. These are shown in **Figure 2** as a function of Ω_{BP} . Values of Ω_{BP} are available from various spectroscopy methods, which unfortunately, do not necessarily probe the full $Z(\omega)$. Hence, average values of Ω_{BP} have been used in **Figure 2**. It is remarkable that **Figure 2** suggests a relation between Ω_{IR} and Ω_{BP} for all these various glasses, and that those glasses having a strong to intermediate excess of modes seem to obey $\Omega_{IR} \approx \Omega_{BP}$, in agreement with [3].

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Principal Publication and Authors

B. Rufflé (a), G. Guimbretière (a), E. Courtens (a), R. Vacher (a) and G. Monaco (b), *Phys. Rev. Lett.* **96**, 045502 (2006).

(a) LCVN, Université Montpellier 2 and CNRS (France)

(b) ESRF