Phase transitions of $LaTiO_3$ under pressure

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The family of Ti-based $RTiO_3$ compounds, where R stands for a rare-earth ion, crystallize in the $GdFeO_3$-type perovskite structure (SG *Pnma*, *Z*=4) at ambient conditions [1]. They all have a single electron in the t_{2g} orbitals of the Ti 3*d* shell (Ti^{3+}) and are all Mott insulators [2,3]. Upon decreasing the ionic radius in the rare-earth series from La to Y, the structural distortions increase and, consequently, the one-electron bandwidth gets smaller [2,3]. $LaTiO_3$ exhibits the smallest structural distortions among the series and, concomitantly, has the smallest optical band gap (E_g~0.1 eV [1]). The latter implies that $LaTiO_3$ is on the verge of an insulator-to-metal transition. Indeed, previous high-pressure mid-infrared reflectivity investigations [4] detected the onset of an insulator-to-metal transition above 10 GPa.

The pressure-induced metallization motivated us to perform high-pressure x-ray diffraction (XRD) and Raman studies on $LaTiO_3$ in order to detect the response of the structure and the lattice dynamics. From our XRD study, we observe an *isostructural* transition taking place at ~10 GPa which coincides with the metallization of the compound. Upon further compression, the orthorhombic *Pnma* phase transforms into a tetragonal *I*4/*mcm* structure above 30 GPa. High-pressure Raman studies at ambient and low temperatures are consistent with the XRD results. We have observed an unusual enhancement of the Raman intensity upon entering the metallic state; a possible explanation of this peculiar behavior in terms of electronic correlations is offered.

References

[1] D. A. Crandles, T. Timusk, J. D. Garrett, and J. E. Greedan, Phys. C **201**, 407 (1992).
[2] M. Mochizuki and M. Imada, New J. Phys. **6**, 154 (2004) and references therein.
[3] E. Pavarini, A Yamasaki, J Nuss, and O K Andersen, New J. Phys. 7, 188 (2005) and references therein.
[4] I. Loa, X.Wang, K. Syassen, M. Hanand, T. Lorenz, H. Roth, and Y.-L. Mathis (unpublished).