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Structure and dynamics in photovoltaic metal hydrides

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Solar cell technology is an active area of research with the quest to improve the efficiency of solar cells to above the current value of 44% [1]. Hot carrier solar cells are particular types of cells which may enable higher efficiencies to be obtained. However, these are only feasible where there is a sufficiently large band gap in the phonon dispersion of the bulk material to minimise energy loss to from thermalisation, thus keeping the electrons 'hot'. Binary compounds with a large mass difference between the two constituent atoms, and high level of crystal symmetry such as titanium hydride, can have such a gap in their phonon dispersion.
Titanium hydride is an interesting photovoltaic material with a broad range of properties, which vary depending on the proportion of hydride present. Theoretical studies show TiH2 has a phonon band gap of 95 meV in the bulk phase [2], however, there is little experimental data to confirm this. TiH1.65 has been measured using X-ray powder diffraction and inelastic neutron scattering whereby it was found that this sample had a phonon band gap of 65 meV [3].
We present here further X-ray powder diffraction and ineleastic neutron scattering data on powder samples of TiH2 and TiH1.5 whereby we show the correlation of phonon band gap with hydrogen content.

[1] Solar cell efficiency graph https://phys.org/news/2016-02-solar-cell-efficiency-nrel.html (last accessed 15/09/2018)
[2] K. V. Shanavas, L. Lindsay & D. S. Parker. Sci. Rep. 6 (2016) 28102
[3] P. Wang, G. N. Iles, R. A. Mole, D. Yu, X. Wen, K-F. Aguey-Zinsou, S. Shrestha, G. Conibeer. Jpn. J. Appl. Phys. 56, 08MA10 (2017)

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