MS11-P3 Structure resolution of the complex γ-$La_6W_2O_{15}$

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Oxides in the Ln_2O_3-MO_3 (M = Mo and W) system are of significant technological interest for their laser applications [1], ionic conduction [2], catalytic [3] and ferroelectric [4] properties. The La_2O_3-WO_3 phase diagram has been studied by a number of groups [5-7], but little detailed crystallographic information was reported due to the lack of good single crystals. Some of the reported compositions have not been appropriately characterized. Recently, the structures of La_2WO_6, $La_{18}W_{10}O_{57}$ and $La_{10}W_2O_{21}$ were solved using X-ray powder diffraction (XRPD) [8-10]. For the $La_6W_2O_{15}$ compound phase transitions at 630 and 930°C have been reported [1-3]. The structure of the high temperature phase α-$La_6W_2O_{15}$ was determined ab-initio by XRPD using direct methods [11]. The lower-temperature forms β and γ, however, couldn't be determined due to the large number of reflections in the X-ray powder diffraction pattern and the relatively low symmetry of the system. The existing literature on γ-$La_6W_2O_{15}$ only relates two sets of unit cell parameters [5-6], that almost match the XRPD pattern of γ-$La_6W_2O_{15}$, but some weak peaks remain without indexation and can't be explained by the presence of any impurity.

Here we present the combination of XRPD and electron diffraction studies to solve the complex structure of γ-$La_6W_2O_{15}$. From standard selected area electron diffraction the unit cell was determined to be monoclinic with cell parameters a=1.56 nm, b=1.21 nm, c=1.47 nm, β=110°. Due to the low symmetry of the crystal system and the large unit cell, a huge number of reflections needed to be acquired, so that electron diffraction tomography was used to record the intensities. The structure of γ-$La_6W_2O_{15}$ was successfully solved.

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