Rhenium oxide (reo3) and highly applied pressure

1. Describe the symmetry characteristics of the ReO$_3$ polymorphs and their relationship to applied pressure.

Rhenium Oxide also known as ReO$_3$ has been researched and looked into detail widely with the use of highly applied pressure. ReO$_3$ is described as a non distorted structure at surrounding pressure levels. Accurate and precise measurements of the pressure-volume relationship crafted by Batloff showed that the transistion pressure was at a value of 5. 0kbar and also presented that volume strain is related to (P-P$_C$)$^{2/3}$. Differences in volume strain was evidently great when comparing with other materials that went through the same process. The reason for this large difference was due to the buckling of the Re-O-Re bonds while ReO$_6$ continued to be firm and strong. With the assumption that octahedral rotation is always as rigid units, stress on rotations that are small will be directly related to the square of the rotation angle, Ø that leads to Ø^2 . This in turn would allow the polymorph to transform into various phases. The curvature behaviour which was found by Razavi starts at low temperatures with pressure level of 3kbar. M$_3$ phonons being triply degenerate allows the surrounding temperature of ReO$_3$ with a ambient pressure to have a Pm-3m symmetry. At this current stage it will undergo a transition to a structure that contains a Im-3 symmetry. When changed to a tetragonal form, it will be P4/mbm at 5. 2kbar and cubic Im3 at 7. 3kbar at increased levels of pressure. The Im3 structures were formed with the process known as condensation from one, two or three M$_3$ phonons. With this transformation, the cubic structure will go through a rhombohedral phase with the symmetry structure of R-3c. The current R-3c will morph again to a rhombohedral phase. ReO$_6$ being a octahedral undergoes a

distortion at high pressure, giving a rotation angle of (P-PC) $^\beta$ where β= 0. 322(5) (β describes the large critical region where the rotation angle is more than 14º) that is valid from pressure levels of 5. 0 to 27. 4kbar. Pressure measurements are mainly done to identify different high pressure formations of the ReO $_3$ and the quantity of these formations. Particularly with the use of the time of flight Laue method, when the pressure formation reaches a value of 15 kbar, the structure deduced as a cubic Im3. Despite, the discovery there was a downturn which was the values tabulated was only at a single pressure point. Therefore the entire formation of the breakdown of the structured could not be figured out.

0. Describe the metrical relationships between the polymorph unit cells and ReO6 octahedral tilting. Use the CIF files to create ATOMS drawings that support your analysis.

The malformation of perovskite structures can be acquired with reference from the Pm3m structure by rotating the octahedral about the cubic axes. High tension and stress arrangements can be identified and elaborated with the aid of 23 various rotating arrangements that was discovered by Glazer. Respective symmetry groups for high stress transitions include the P4/mbm and Im3 where both groups are homogenous with the M $_3$ phonon condensation. The element Re is fixed in the 8c position in the Im3 space group with only 2 thermal values whereas the oxygen atoms is found to be at the 24g position with 4 thermal values. With a increased in the loading added to the P4/mbm structure will create a deceasing strain that may deform the structure. P4/mbm being a 7 lattice point structure has a normal way of placing the positions of the elements found in ReO3. The Rhenium

element is located in the 2b position while the oxygen atom would be fixated in the 4h and 2a position. In the presence of surrounding atmospheric pressure, the direct dependency of the oxygen atoms is fairly lower in the Im3 group than the one found in the Pm3m. In the Im3 unit cell for the ReO_3, rotation was done around the coordinates of (111) for the eight sided compound. Evidently P4/mbm produces a nonzero seven sided pull that creates a positive and negative strain value. This rotation created the process of condensation that affected all three M_3 phonons. Deformation in the eight sided ReO6 produces two different Re-O bond distances in the P4/mbm formation while there would only be a single Re-O bond found in the Im3 strucutres. Re-O bonds parallel with the c axis will remain in a pressed state when turned whereas Re-O bond that are normal to the c axis will not be in a pressed position but instead arranged in an order where there are gaps. However both formations include double O-O corners of the octahedron that is used to quantify any errors in ReO6. However the O-O distances found in the Im3 and P4/mbm are varied at a pressure value of 27. 40kbar that leads to certain abnormalities but can be ignored as trivial.

0. Explain the distortion of the ReO_6 octahedra with pressure and quantify the ReO_6 octahedral titlting.

The deformation and the distortion of the ReO_6 octahedron is usually found in the P4/mbm and Im3 structures. Starting with the P4/mbm, there are two symmetry Re-O bonds which are not equal in nature. With the process known as the powder neutron diffraction , the results obtained shows the in depth structural details of the transformation with the function of pressure and thus this confirms that at least 2 high pressure phases are present. When the

ReO6 octahedra are rotated they are observed more with ease through the neutrons than the x rays. The method known as Rietveld method of the structural refinement with the high resolution powder data produces the single-crystal neutron diffraction study and this would allow the pressure dependence of the distortion to be measured with sufficient accuracy to state that the order parameter exponent β where Ø is proportional to the $(P-P_c)^{\beta}$ presents the pressure dependence of the rotation angle. This pressure based on the rotation angle is illustrated well by the law of power in the formula $Ø\sim(P-P_c)^{\beta}$. Ø against the pressure and the curve is plotted with this reference. The result from the exponent β was obtained with the linear gradient of the slope of the lnØ against the $\ln(P-P_c)$ curve that produces the value of $\beta= 0. 322(5)$. Through the discrepancies Ø is always continuing with the stress value of 5 kbar despite the direction of the rotation axis that would vary from (100) to (111) during the change from P4/mbm to the Im3 phase (5. 3kbar). With condensation of one, two or three M_3 phonons would increase the phase transition from Pm3m to P4/mbm to I4/mm and lastly to the Im3 that have usually been seen in $Na_x WO_3$ during the M_3 phonon condensation upon cooling. The parameter for the phase transition would be a three component order with the Ø as the magnitude of the rotation angle surrounding the direction of the rotation aixs. The transformation from Pm3m to any of the groups between the P4/mbm, I4/mmm and Im3 would be the first order that would produce from the rotation around a axis. Abnormalities in the lattice during the transformation would have been seen in the $Na_x WO_3$.