

Synthesis of rhenium carbide at extreme P-T conditions

Juarez-Arellano, Erick A.¹ Winkler, Björn¹ Friedrich, Alexandra¹ Wilson, Dan J.¹ Koch-Müller, Monika² Knorr, Karsten³ Crichton, Wilson⁴

¹Institut für Geowissenschaften, Goethe-Universität, Frankfurt am Main ²GeoForschungsZentrum, Potsdam ³Institut für Geowissenschaften / Mineralogie / Kristallographie, Christian-Albrechts-Universität zu Kiel, Kiel ⁴ESRF, Grenoble, France

It is well established that rhenium does not form stoichiometric carbides at ambient pressure. The phase diagram of the system Re-C shows a limited solubility of carbon into rhenium, Hughes (1959). The maximum solubility is reached at 11.7 at.% C at the eutectic temperature (2773 K) and it falls sharply with temperature (4.2 at.% C at 2073 K). No intermediate phase exists. In contrast, at high pressures the formation of rhenium carbides has been reported by Popova et al. (1971, 1972, 1975). They synthesized a hexagonal and a cubic ReC phase ($a = 4.005 \text{ \AA}$) at different P-T conditions. The hexagonal ReC phase was reported to have a γ' -MoC type structure, with lattice parameters $a = 2.8403 \text{ \AA}$, $c = 9.8543 \text{ \AA}$, obtained at synthesis conditions above 6 GPa and 1073 K. No further structural details were given for either the hexagonal or for the cubic ReC phases. However, all these measurements were performed on quenched samples using X-ray diffraction. This implies that rhenium carbide phases which might only be stable at high (P-T) conditions would not have been detected. Therefore, to further investigate the reaction of rhenium with carbon, we undertook laser heated diamond anvil cell experiments, multi-anvil press synthesis experiments and density functional theory (DFT) based model calculations.

Our results provide strong evidence for a reaction of Re and carbon at extreme P-T conditions. A hexagonal ReC_x was identified as the stable phase at high-(P,T) conditions. A composition of $\text{ReC}_{0.5}$ is proposed. No evidence for a cubic ReC polymorph with rocksalt structure, as suggested in the literature, or for any other phase was found at the P-T conditions explored. A preliminary P-T rhenium-carbon phase diagram has been derived and properties such as bulk moduli and elastic stiffness coefficients were obtained.

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submitted by: **Juarez-Arellano, Erick**

email: **arellano@kristall.uni-
frankfurt.de**

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