

Phase change
MoC

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A New Phase formed by High-Pressure Treatment: Face-centred Cubic Molybdenum Monocarbide

The attempted preparation and retention of polymorphs dependent on pressure is an important area of high-pressure research. Some of these phases are found in Nature; others were unknown prior to the recent development of equipment suitable for research at high pressure and high temperature.

Although high-pressure phases are thermodynamically unstable at ambient conditions, a few have been retained by quenching to room temperature under pressure. High-pressure polymorphs found in the Earth's crust¹ include several minerals, for example, the pyroxene jadeite, $\text{NaAlSi}_2\text{O}_6$ (ref. 2); kyanite, Al_2SiO_5 (ref. 3); and diamond (ref. 4). Previously unknown phases are coesite², a form of SiO_2 with a higher density than quartz; borazon³, a cubic form of boron nitride; and several compounds of the garnet type¹. A number of high-pressure polymorphs of pure metals, which unlike the above compounds cannot be retained at ambient conditions, have been reported⁷.

High-pressure experiments on the molybdenum-carbon system have revealed a new form for the monocarbide phase. The new form, designated α -MoC, has been retained to atmospheric pressure. Synthesis was achieved from both an equiatomic mixture of molybdenum and carbon and an equiatomic mixture of the compound Mo_2C and carbon at pressures and temperatures in the range of 40–70 kilobars and 1,800°–2,500° C. The X-ray diffraction pattern for α -MoC showed the first ten lines for a face-centred cubic structure. No additional lines were observed. The average lattice parameter was $a_0 = 4.27 \text{ \AA}$. In addition to high-pressure experiments in which the only product was α -MoC, other experiments carried out at lower temperatures and pressures afforded evidence for all the phases reported⁸ for the molybdenum-carbon system at atmospheric pressure. A summary of the lattice parameters of the various phases is given in Table 1.

Further experimental detail and a thermodynamic analysis of the effect of pressure on the equiatomic region of the molybdenum-carbon system will be published elsewhere.

Table 1. COMPOSITION AND DIMENSIONS OF PHASES IN THE MOLYBDENUM-CARBON SYSTEM

Com- position	Symbol	Structure	X-ray data			Molybdenum atoms/unit cell
			$a_0(\text{\AA})$	$c_0(\text{\AA})$	c_0/a_0	
Mo ₄ C	β	hexagonal closest packing	3.002	4.724	1.574	2
MoC	γ	hexagonal	2.898	2.809	0.969	1
MoC	γ'	hexagonal	2.932	10.97	3.742	4
MoC	η	complex hexagonal closest packing	3.00	14.58	4.86	6
MoC	α	face-centred cubic (sod- ium chlor- ide)	4.27	—	—	4

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