Phase change

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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 crust[1] include several minerals, for example, the pyroxene jadeite, $NaAlSi_2O_6$ (ref. 2); kyanite, Al_2SiO_5 (ref. 3); and diamond (ref. 4). Previously unknown phases are coesite[5], a form of SiO_2 with a higher density than quartz; borazon[6], a cubic form of boron nitride; and several compounds of the garnet type[1]. A number of high-pressure polymorphs of pure metals, which unlike the above compounds cannot be retained at ambient conditions, have been reported[7].

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 $a_0 = 4{\cdot}27$ Å. 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 reported[8] 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.