structure transitions of boron in megabar shock compression-UNLOADING cycle

Molodets A.M.

Institute of Problems of Chemical Physics RAS,Moscow, Russia, [molodets@icp.ac.ru](mailto:molodets@icp.ac.ru)

Studies of the physics of boron at high pressures have been intensively conducted for many years (see references in [1–4]). It was found that the solid phase of boron exists in the form of several crystalline modifications, as well as in the amorphous state. The boric icosahedron with twelve atoms at the vertices and twenty triangular faces is the main structural unit of most allotropes of the solid phase of boron. The region of higher pressures of ~100 GPa (megabar region) is of increased interest due to the fact that in this extreme region, a change in the structural unit of the “low” pressure - boron icosahedron with the formation of the “atomic” alpha-B (Ga) phase occurs. Until recently, studies of boron transformations in the megabar region were theoretical, but recently experimental work using static pressure diamond anvils with heating [1] and using high pressures and temperatures of shock-wave compression appeared. In this report, some results of the study of the structural transformations of boron at high shock compression pressures are presented.

Measurements of the electrical conductivity of polycrystalline boron samples β-B106 under shock compression [2] suggest that in the dynamic pressure range of 90–110 GPa and shock temperatures of 700–800 K, polycrystalline boron β-B106 is amorphized. This assumption is confirmed in experiments on the recovering of shock-pressed samples of boron [3]. X-ray diffraction study of samples of polycrystalline beta-rhombohedral boron after shock wave exposure to pressures of 115 (5) GPa and temperatures of ~ 800-1400 K reveals the presence of *am*B amorphous phase. However, in addition to the amorphous component, the conversion products also contain a tetragonal modification of boron T-B192.

In general, comparing the results of [1] and our results, we can state the following. The products of the transformation of the rhombohedral phase of β-B106 in the region of the existence of a “non-icosahedral” phase of boron under the same pressure 115 (5) under static and dynamic conditions are different: in [1] the formation of the “nonicosahedral” modification α-B (Ga) is observed, and in [3] the final conversion products are *am*B and T-B192. In this paper, the details of the route of boron transformation under shock compression are discussed. At the initial part of the phase trajectory of the stepped shock compression up to 10–30 GPa, rhombohedral boron β-B106 remains in a metastable state not only when crossing the equilibrium lines β-B106↔α -B12 and α-B12↔γ-B28, but also in the region of the rhombic boron γ-B28 at 30–90 GPa. However, further amorphization occurs as β-B106→*am*B, where *am*B is "icosahedral" (in the sense of [4]) amorphous boron A1-B106 Then, in a discharge wave at pressures of 20-30 GPa and temperatures of ~800 K, part of amorphous boron A1-B106 turns into beta-B106 and, finally, at pressures of 10 GPa, the final transformation of beta-B106→T-B192 occurs.

This work was supported by the RFBR grant No. 19-08-00561.

References

1. Chuvashova I. et.al., Physical Review B. 95, 180102(R) (2017).
2. Молодец А.М. и др. Физика твердого тела. 59, вып. 7, 1379 (2017).
3. Молодец А.М. и др. ПЖЭТФ.108, вып. 6, 430 (2018).
4. An Q. et al., Physical Review B. 95, 064108 (2017).