SHOCK-INDUCED PHASE TRANSFORMATIONS AND THEIR NANOSCALE RECORD

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Background: Ever since Hugoniot parameters are measured in shock experiments it is known that minerals undergo high-pressure phase transitions. The nature and mechanism of these phase changes are however not obvious from Hugoniot data and require (electron) microscopic examination of recovered phases [1]. Microscopic observations show, for example, that naturally shocked quartz rarely contains any stishovite, although it is still widely assumed that quartz converts completely to stishovite under shock compression, which then largely reverts back to the amorphous state [2]. In the short time frame of shock, a solid-state transformation is however implausible due to its reconstructive nature, which requires atomic diffusion and change in coordination of silicon from tetrahedral to octahedral. This contribution aims at discussing "plausible" mechanisms of high-pressure phase transformations in shock events on the basis of microstructural evidence.

Liquidus crystallization: In case of coesite and stishovite, transmission electron microscopy (TEM) has shown that these high-pressure silica polymorphs occur as tiny (<<1 μm) crystals or polycrystalline aggregates in silica glass [3, 4], either in diaplectic glass or in shock veins or pockets. These regions are hot spots in impact rocks, where temperatures are sufficiently high to melt quartz under shock compression. Coesite and stishovite may then crystallize from melt during the release paths, which pass through their stability fields. As consequence of fast cooling, the nucleation rate is high and crystals are very small. In strong support of the rapid liquid-crystallization hypothesis is the almost defect-free microstructure of the high-pressure phases. The formation of high-pressure silicates from melt occurs generally at very high temperatures (> 2000 °C) and is thus not kinetically inhibited.

The liquidus crystallization of even more complex high-pressure silicates (e.g. lingunite, wadsleyite, ringwoodite, akimotoite, bridgmanite) is also a well known phenomenon in shock veins of strongly shocked meteorites [5]. The resultant high-pressure phases are generally devoid of shear-induced imperfections and can only contain growth defects such as {110} stacking faults in ringwoodite.

Solid-state transformation: Recent advances have also been achieved in understanding high-pressure polymorphic transitions of durable minerals that operate in the solid state by diffusionless shear mechanisms. Examples of such martensitic phase transitions are (1) post-rutile transitions to α-PbO_2 and baddeleyite-structured (akaogiite) titania polymorphs [6], (2) the zircon-to-reidite transition [7], and (3) the transition of ilmenite to a $LiNbO_3$-structured phase [6].

These phase changes can be envisaged as shear-induces transitions between close-packed crystal structures. For example, the rutile structure can be described as consisting of hexagonal-close-packed oxygen atoms with titanium atoms occupying half the close-packed rows of octahedral interstices [1]. A cooperative movement of titanium atoms by ½ $[01\bar{1}]$ shear on alternate (011) oxygen planes transforms rutile into the α-PbO_2 structure. In reality, the short timescale of shock compression impedes this perfect motion, explaining why shock-transformed rutile commonly contains numerous planar defects on {011}.

Similar planar defects parallel to {100} planes are known to occur in zircon. These defects play a major role in the transformation of zircon to reidite (scheelite-structured). The atomic positions of Zr and Si in the zircon structure are shifted to the positions expected in reidite by ¼ <010> glide on the {100} planes. After this martensitic shear mechanism displacive rotations of oxygens around the cations fully convert the zircon structure into the scheelite structure [8]. This results finally in an epitaxial relationship between zircon (Zr) and reidite (Rei) with $\{100\}_{Zr}//\{112\}_{Rei}$ and $[001]_{Zr}//\langle110\rangle_{Rei}$.

Conclusions: Despite the high speed of shock processes minerals can convert to high-pressure polymorphs by two mechanisms: (1) liquidus crystallization and (2) martensitic shear. Defect-free polycrystalline aggregates of tiny crystals are often indicative of liquidus crystallization. Martensitic mechanisms apparently operate predominantly in close-packed structures with simple compositions and result in distinct lattice defects such as partial dislocations and stacking faults.

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