Crystal-Amorphous and Crystal-Crystal Phase Transformations via Virtual Melting

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Pressure-induced crystal (c)-amorphous (a) phase transformations (PTs) were considered in literature (e.g. for ice, guartz, high albeite, and jadeite) as a low temperature analog of melting along the metastable continuation of melting lines in pressure-temperature phase diagram. However, some contradictions were found concerning metastable melting hypotheses [1]. In this paper, a new mechanism of pressure-induced c-a and c-c PTs and internal stress relaxation via virtual melting (VM) induced by internal stresses was justified thermodynamically and kinetically. The energy of the internal elastic stresses, induced by large transformation strain for c-c PT, increases the driving force for melting and reduces the melting temperature; under certain conditions, a barrierless melt nucleation occurs. Melting releases the internal stresses and the unstable melt solidifies into the stable crystalline (above the glass transition temperature) or amorphous (below the glass transition temperature) phase. A short-lived unstable melt (transitional state) is called the VM [2]. VM removes interface friction, reduces kinetic barrier, increases atomic mobility, can reduce thermodynamic melting temperature and stabilize subcritical c nucleus or transform it to an amorphous nucleus. VM also resolves the contradictions mentioned in literature [1]. We combine VM, detailed stress analysis and nonequilibrium PT diagrams to develop new scenarios of c-a and c-c PTs. Results are applied for a new interpretation of melting, c-c and c-a PT mechanisms in ice Ih. VM is expected to be a main mechanism of amorphization in geological materials (e.g. α -quartz, coesite, and jadeite), in brittle semiconductors (e.g. Ge and Si), in materials leading to superhard phases (e.g. BN and graphite), as well as polymet, Zn₄₃Sb₅₇ and Cd₄₃Sb₅₇.

1. V.V. Brazhkin, A. G. Lyapin. High Pressure Research. 1996, vol. 15, 9-30.

2. V. I. Levitas, B. F.Henson, L. B. Smilowitz, B. W. Asay. Phys. Rev. Lett. 2004, vol. 92, 235702.