Phase transition of SiGe alloys under high pressures and high temperatures

*Riping Liu⁹⁶⁵² and Xinyu Zhang⁹⁸³³

Key Lab of Metastable Materials, Yanshan University, P.R.China

The Si_{1-x}Ge_x alloys have attracted a great deal of attention lately due to its importance in new electronic and optical devices. Both Si and Ge are covalent crystals, which display a semiconductor to metal transition under high pressure. The Si_{1-x}Ge_x alloys constitute an ideal mixed crystal system. At ambient pressure, it crystallizes in the cubic-diamond structure, with Ge and Si atoms distributed randomly among the lattice sites. Only a few studies of the behavior of this alloy have been carried out under pressure. The studying of phase transformations under pressure in both Si and Ge has been an extremely active field since the discovery of the cubic-diamond to beta-tin phase transformation almost a half century ago.

The in-situ X-ray diffraction investigation under high pressure and high temperature was carried out in SPring-8 to study the solidification behavior of this alloy under high pressure and the possibility to keep the high pressure metallic metastable phase after decompression. The following results were obtained in the present study.

- 1. The "P-T" phase diagram of Si_{1-x}Ge_x alloy moves right and up according to that of pure Ge by alloying effect of Si element. Fig 1 shows the Si₅₀Ge₅₀ alloy kept cubic diamond structure from room temperature to melt point under 8.79GPa pressure.
- 2. The cubic diamond structure phase was kept after quenching the Si₅₀Ge₅₀ and Si₂₅Ge₇₅ alloys melt when the pressure was smaller than 9GPa. But under 9.5GPa, quenching the Si₂₅Ge₇₅ melt caused formation of mixtures of some phases including cubic diamond structure phase, β -tin structure

phase and GeIII phase. We resume that there is a critical pressure around 9 GPa under which the metallic high pressure metastable phases could be kept. During decompression the mixtures of some phases changed to the cubic diamond structure phase

3. The diffraction data of Si₅₀Ge₅₀ were collected during cooling continuously under 8.8GPa and 6.3GPa respectively. The Si₅₀Ge₅₀ alloy sample solidified and formed the cubic diamond structure phase when cooling. But the grains of the samples grew into big sizes easily, only a small quantity of peaks of sample were recorded.

The metallic metastable phases of SiGe alloy could not be obtained by quenching or cooling under the pressure below 9 GPa. And the transformations cubic diamond to high pressure forms did not occur. But the high pressure metallic phases are expected to be obtained after quenching or cooling down from melt under high enough pressure.

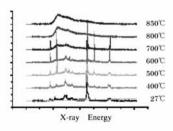


Fig.1 Variation of x-ray diffraction profiles of Si50Ge50 alloy with increasing temperatures at 8.79 GPa

XAFS study of pressure-induced changes in Ge-Sb-Te layers used for near-field optical recording below the diffraction limit

P.Fons† (0007309), A. Kolobov†* (0007323), Y. Katayama(0001214)[§], J. Tominaga† † CANFOR (AIST), §JASR

Te-based alloys, in particular, Ge-Sb-Te (GST) and Ag-In-Sb-Te (AIST) alloys are widely used in production of phase-change media such as re-writable CDs and DVDs. Recently it has been demonstrated that these materials can also be used for near-field optical recording in super-resolution near-field structure (super-RENS) optical discs.

An important difference between presently used phase-change media and super-RENS is that in the latter both recorded and non-recorded areas are crystalline. The difference between the recorded and non-recorded areas in super-RENS is that under the recorded bit there is a bubble formed by laser-induced (thermal) decomposition of a Pt-oxide. During decomposition the GST layer is also heated and additionally exposed to pressure. We have argued recently that this transformation, which is likely to be of a ferroelectric nature, may be a key point in super dense optical recording. To investigate the structural changes, we have performed extended x-ray absorption fine

performed extended x-ray absorption fine structure (EXAFS) measurements on GST subjected to the simultaneous action of temperature and pressure at BL14B. The samples were 3-micron thick GST layers deposited on Kapton. Prior to the experiment, the GST layers were crystallized by annealing for 3 hrs, at 150°C in Ar. A stack of layers was put into a high-pressure cell using standard procedures. Measurements were performed at room temperature and at 550°C (somewhat lower than the decomposition temperature of Pt-oxide) for pressures up to 10 GPa.

Fig. 1 shows the variation of the Ge-Te bond length with pressure. One can see than in the starting structure there are two different Ge-Te distances that merge together at a pressure of ~3 GPa after which the Ge-Te distance decreases monotonically.

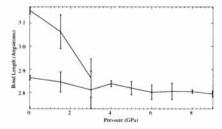


Fig 1. Fitted bond-lengths as a function of pressure

In the case of high-temperature measurements, the amplitude of the Fourier transform is significantly modified indicating a major structural change. Curve-fitting analysis is currently underway.