Polymorphism and metastable phenomena in liquid Sn under pressure

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Polyamorphism, the property of liquids and glassy systems of transforming between different structures in response to the pressure and the temperature, has been proposed and discussed for a variety of systems.

This is a fundamental phenomenon with strong interdisciplinary implications ranging from earth and planetary science to chemistry and material science. However, very few experiments have been performed so far, especially for simple substances.

Within this contribution, we report about new experimental results on liquid and undercooled tin under high-pressure obtained by combining x-ray absorption spectroscopy (XAS) and x-ray diffraction.

The interest in liquid Sn stems from the possible occurrence of liquid-liquid phase transitions which have been related to the soft-core interaction potential often used to describe not-simple liquid metals, such as Sn, Bi, Ga or Ge. In addition, discontinuities of volume, heat capacity and electric resistivity have been reported for Sn in a rather narrow interval of the pressure- temperature phase diagram.

We investigated Sn at high-pressure up to 4 GPa and temperature up to 700 K by a combination of experimental techniques such as x-ray absorption spectroscopy, fixed energy x-ray absorption temperature scans and energy scanning x-ray diffraction.

We show that crucial properties like undercooling limit and local structure change upon application of pressure. In particular, above a critical pressure (≈ 2 GPa) the undercooling limit of liquid tin is drastically reduced by preferential nucleation of the liquid into a solid phase (Sn-III) stable only at much higher pressures (≈ 3 GPa). This phenomenon is accompanied by a gradual change of the local structure, analyzed on the basis of a threedimensional structural model compatible with XAS data. The picture emerging from this study of liquid Sn is that of a liquid composed of tetrahedral and close-packed configurations, where the latter dominate at high pressures leading to preferential nucleation toward a phase of higher coordination (Sn-III) as the pressure increases.

No evidence for a definite liquid-liquid phase transition was found, but a clear experimental proof of a drastic change in the nucleation properties at high pressures, accompanied by a change of the short-range local geometrical ordering of the liquid has been provided.