

Dynamics of the Negative Thermal Expansion in Tellurium based liquid alloys

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We measured on IN6 (ILL) the vibrational properties of some liquid Te-based covalent systems. The aim of this experiment was to study the behavior with temperature of two different kind of systems: Te-rich Germanium Telluride (GeTe₆, which is the eutectic composition, and GeTe₁₂), and phase change materials (Ge₁Sb₂Te₄ and Ge₂Sb₂Te₅). This study was guided by the technological interest of the phase change material, but also by the wish to study a phenomenon as fundamental as the Peierls distortion, which takes place in those covalent systems.

We showed that the phase change materials don't have any variation of their vibrational density of states with temperature, while in both other compounds we noted a pronounced change while increasing temperature. The Te-rich binary systems are known to show a density anomaly with temperature around the melting point. The evolution we observed in the vibrational density of states, compared to the constant behavior of phase change materials, is related to this anomaly.

In addition, we show ab initio calculations results that were obtained for GeTe₆, and that are in qualitative agreement with neutrons experiment.

References

Raty J.-Y., Godlevsky V., Ghosez P., Bichara C., Gaspard J.-P., Chelikowsky J. R., *Evidence of a reentrant Peierls distortion in liquid GeTe*. Phys. Rev. Lett., 85, -9-, 1950-3, 2000.

Bergman C., Bichara C., Gaspard J.-P., Tsuchiya Y. *Experimental investigation of the water-like density anomaly in liquid Ge₁₅Te₈₅ eutectic alloys*. Phys. Rev. B67, 104202, 2003.

Coulet M.-V., Testemale D., Hazemann J.-L., Gaspard J.-P., Bichara C., *A Reverse Monte Carlo analysis of the local order in liquid Ge₁₅Te₈₅ alloys combining neutron scattering and X-Ray Absorption Spectroscopy*. Phys. Rev. B, 72, 174209, 2005.

Bichara C., Johnson M., Raty J.-Y., *Temperature-induced density anomaly in Te-rich liquid germanium tellurides: p versus sp³ bonding?* Phys. Rev. Lett., 95, 267801, 2005.

C. Bichara, M. Johnson, J.-P. Gaspard, *Octahedral structure of liquid GeSb₂Te₄ alloy : first principles molecular dynamics study*, Phys. Rev. B 75, 060201R, 2007.