MATERIALS AT HIGH TEMPERATURE STUDIED BY ULTRAFAST X-RAY ABSORPTION SPECTROSCOPY

P.A. Heimann, S.L. Johnson, A.M. Lindenberg, A.G. MacPhee and R.W. Falcone,

Advanced Light Source, Lawrence Berkeley National Laboratory Department of Physics, University of California at Berkeley

Time-resolved x-ray absorption spectroscopy provides information about the structure and electronic structure of a transient state induced by a laser pulse. The x-ray absorption near edge structure (XANES) is especially sensitive to the electronic structure of the material. Picosecond time resolution allows the spectroscopic measurement of a material at high temperature and near solid density before it undergoes significant expansion. Excited by a femtosecond laser pulse, a sample foil is probed in transmission by the focused broad bandwidth x-rays. A dispersive spectrometer measures an entire x-ray absorption spectrum simultaneously.

Solid covalently bonded semiconductors are known from molecular dynamics calculations to form liquids, which have both metallic and covalent bonding [1]. However, there has been little experimental confirmation of this description of the structure and bonding of melted semiconductors. We have measured the L-edge x-ray absorption spectra of liquid silicon and carbon. For comparison with liquid silicon, molecular dynamics simulations have been performed to determine atomic positions. Then, the x-ray absorption was calculated with the abinitio x-ray scattering code FEFF [2]. The calculations show good agreement with the experimentally measured absorption spectrum of liquid silicon. The properties of liquid carbon are interesting for astrophysical reasons because carbon is an important constituent of some planets. The x-ray absorption spectrum of liquid carbon indicates a transition in bonding from the predominant sp² bonding of soft amorphous carbon to bonds with increased π character.

References

1. I. Stich, R. Car and M. Parrinello, Phys. Rev. Lett. 63, 2240 (1989).

2. A.L. Ankudinov, B. Ravel, J.J. Rehr and S.D. Conradson, Phys.Rev. B 58, 7565 (1998).