Structure of WSi_n cage clusters probed by x-ray absorption fine structure spectra

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Transition metal -encapsulated Si cage clusters are expected to be able to stabilize Si cage structures which are promising building blocks for the fabrication of various nano- and optoelectronics devices [1]. We combined EXAFS and XANES to study the geometric arrangement of W around Si atoms in a series of WSi_n cluster samples. The EXAFS results show similar radial distributions around W atoms in the WSi_n samples and amorphous W-Si alloy, but the spatial distributions in the WSi_n clusters and amorphous W-Si alloy quite different as revealed by detailed multiple-scattering XANES analysis. It is found that WSi_8 and WSi_{12} cage clusters coexists in the as-deposited WSi_n samples. The average fraction of WSi_{12} cluster is evaluated to be 25%, 43%, and 45% for samples deposited in a SiH_4 pressure of 5, 0.5, and 0.1 Pa, respectively.

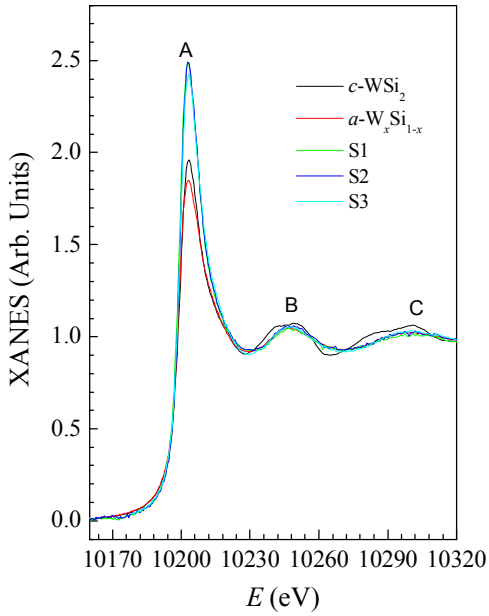

Fig. 1 The normalized XANES spectra of WSi_n samples, *c*-WSi_2 and *a*-W_xSi_{1-x} references. Much stronger white-line peaks for the WSi_n samples than those of *c*-WSi_2 and *a*-W_xSi_{1-x} can be observed.

References

[1] H. Hiura, T. Miyazaki and T. Kanayama: *Phys. Rev. Lett*. **86**, 1733-1736 (2001).