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Nanocrystals and small clusters investigated by synchrotron radiation and microfluidics

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We describe *in-situ* XAS studies using microfluidics to demonstrate its capability, through a couple of applications, the structural and kinetics studies during the initial stage of CdSe nano particles (NPs) and copper small cluster (SCs).

1 Introduction

The past two decades have witnessed an explosive expansion of research on semiconductor nanoparticles (NPs), due to their size-dependent properties and applications in a variety of fields such as solar cells, light emitting diodes, and biological imaging. In this report, we demonstrate that the time-dependent x-ray absorption spectroscopy measured with a microfluidics is advantageous in sensitivity and key information on NPs (size and density) is available in addition to local structure (bond length, coordination number and relative displacement).

2 Experiment

The basic idea is to measure fluorescence XAS by means of position-dependence recorded at different positions along a laminar flow of a reactor channel. A constant velocity flow conveys a small volume of dilute solutions mixed prior to the injection to the reactor which creates nuclei upon heating that grows into the NPs and small clusters (SCs) as a function of time [1].

3 Results and Discussion

We have calculated XANES spectra for the model *n*-atom clusters (*n*=13-135) and found that the experimental data (Figure 1)) is well reproduced by a SC with *n*=13. The MS calculation showed that the characteristic double-peak near-edge features (B, C) around 9000 eV appear only when *n* exceeds 43. As SCs ($n \leq 19$) have a single peak at this energy, the first peak feature around 9000 eV can serve as a signature of a SC ($n \leq 19$). Fig. 1 compares experimental XANES for the Cu SC with the theoretical calculation on a 13-atom model cluster, where (a) and (b) correspond to raw and derivative spectra, respectively. In the 13-atom SC which has a large optical gap, our DFT calculations found that 12 surface atoms are positively charged and have a strong interaction with a ligand amine molecules firming a microscopic electric double layer, distinguished with previously reported clusters.

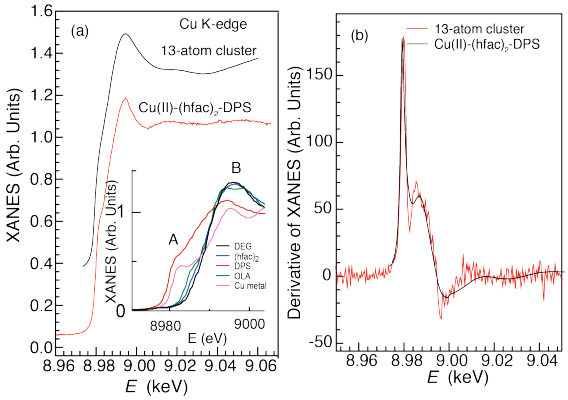

Fig. 1: Cu XANES raw and derivative spectra for Cu SC.

References

[1] H. Oyanagi *et al*. J. Appl. Phys. 111, 084315 (2012).