Three dimensional modeling of *i*-AlCuFe quasicrystal structure from X-ray Absorption Spectroscopy

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Introduction

Quasicrystals (Qcs) are materials with long-range order, but with no three-dimensional translational periodicity. Quasicrystals are known to have unique structural characteristics, and also exhibit unusual physical properties. Although significant progress has been made in determining the atomic structures of diverse QCs, their detailed atomic structure are still far from completely understood. For a detailed description of the three dimensional (3D) structure of the icosahedral $Al_{65}Cu_{23}Fe_{12}$ QC, the multidimensional interpolation approach for quantitative local structure parameter refinement from HERFD XANES and EXAFS was used. The theoretical model of the local environments of copper and iron in the i-$Al_{65}Cu_{23}Fe_{12}$ QC was proposed from the approximant crystalline phase.

Methods

The powder of nominal composition $Al_{65}Cu_{23}Fe_{12}$ was purchased from Sigma-Aldrich. The *i*-$Al_{65}Cu_{23}Fe_{12}$ QC was investigated using X-ray diffraction (XRD), scanning electron microscopy (SEM), Mössbauer spectroscopy, X-ray absorption spectroscopy (HERFD XANES and EXAFS) and X-ray photoelectron spectroscopy (XPS). Experimental Fe K- and Cu K-edge HERFD-XANES and EXAFS spectra were measured at ID-26 beamline of ESRF. Local atomic structure parameters were refined through the fitting of XANES spectra using a multidimensional interpolation approach (FitIt code). The Fe and Cu K-edge XANES spectra and density of states (DOS) were simulated by the full multiple scattering code FEFF9.0.

Results and discussion

The XRD analysis revealed the presence of icosahedral AlCuFe quasicrystal, cubic β-Al(Cu, Fe) phases and a small amount of other crystalline phases. The icosahedral quasicrystalline (i) phase was the major phase for this alloy composition. The second major phases were cubic β-Al(Cu, Fe) phases with the crystal structure of cubic CsCl type. The room temperature Mössbauer study revealed the presence of four doublets that indicates the four nonequivalent iron positions corresponding to the iron on the surface, in the cubic β-Al(Fe), and two others types of local environments in the icosahedral quasicrystalline phase. The 3D structure and local atomic structure parameters (interatomic distances Fe-Al, Cu-Al, Cu-Cu) were refined through the fitting of HERFD XANES spectra using a multidimensional interpolation approach. The density of states (DOS) of the theoretical *i*-$Al_{65}Cu_{23}Fe_{12}$ model was simulated and discussed.

Conclusions

The theoretical model of the local environments of iron and copper in the *i*-$Al_{65}Cu_{23}Fe_{12}$ quasicrystal were built by fitting the Fe K- and Cu K- HERFD XANES and EXAFS spectra. The XPS valence band spectrum was shown to contain density of states of both the icosahedral AlCuFe quasicrystal and cubic β-Al(Cu,Fe) phases. The theoretical model of the *i*-$Al_{65}Cu_{23}Fe_{12}$ quasicrystal fully describes the experimental data.

The study was financially supported by the Ministry of Education and Science of the Russian Federation for the award of grant 16.3871.2017/4.6.